

Supporting Information

***Rec. Nat. Prod.* 20:2 (2026):e25093648**

Bioactive compounds from the flowers of *Cannabis sativa* L.: Isolation of a new alkaloid and biological evaluation of cannabinoids and sesquiterpenoids

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1. Spectroscopic data for compound 1

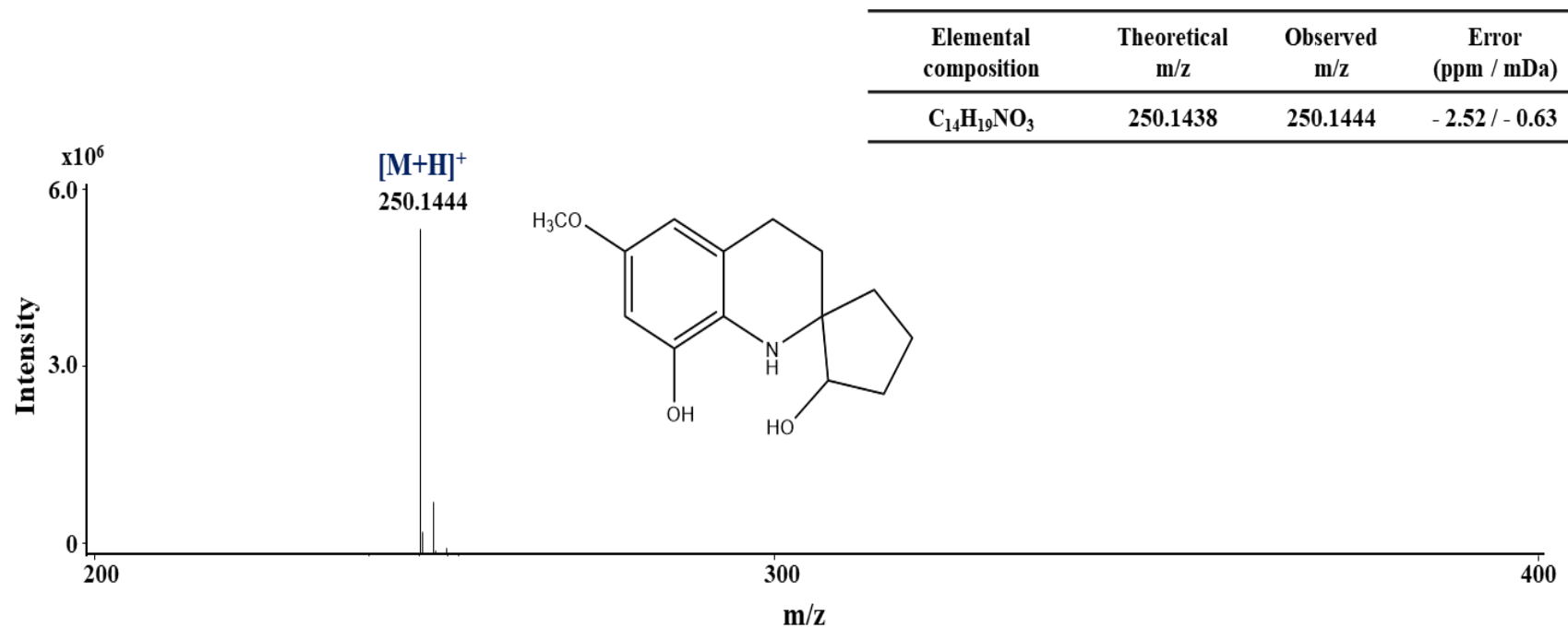


Figure S1. MS spectrum of **1**

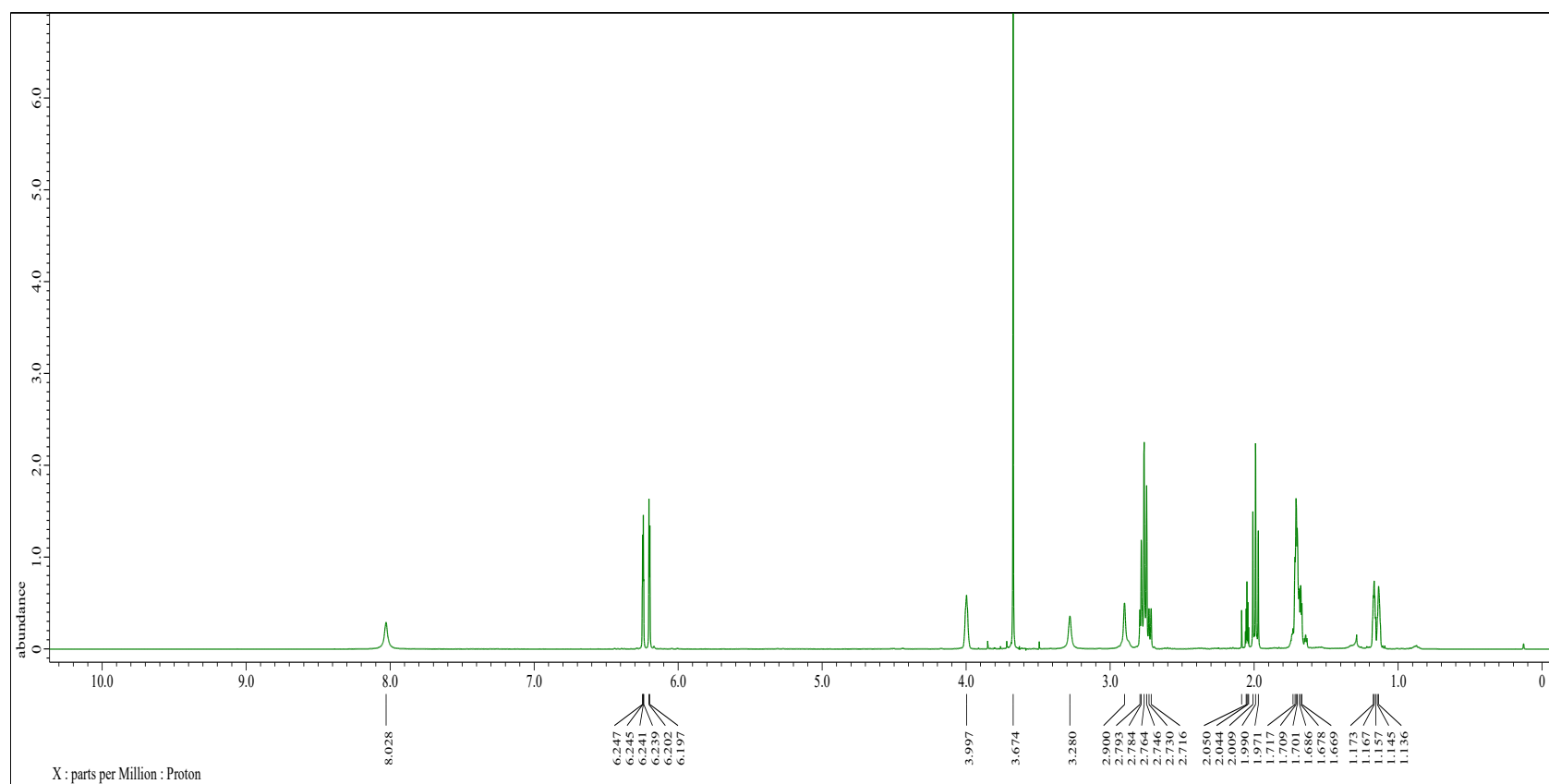


Figure S2. ^1H NMR spectrum of **1** (Recorded in Acetone- d_6)

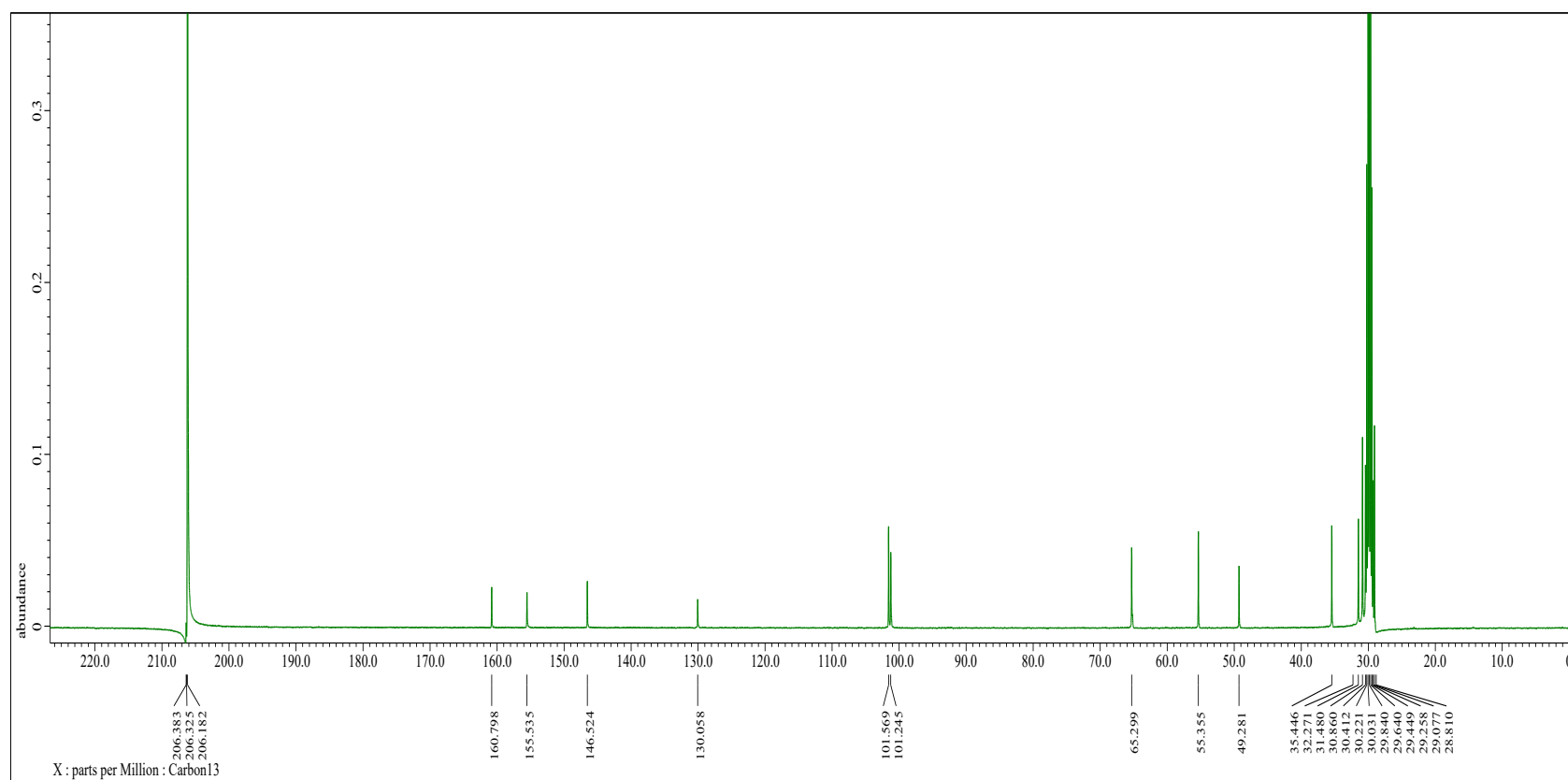


Figure S3. ^{13}C NMR spectrum of **1** (Recorded in Acetone- d_6)

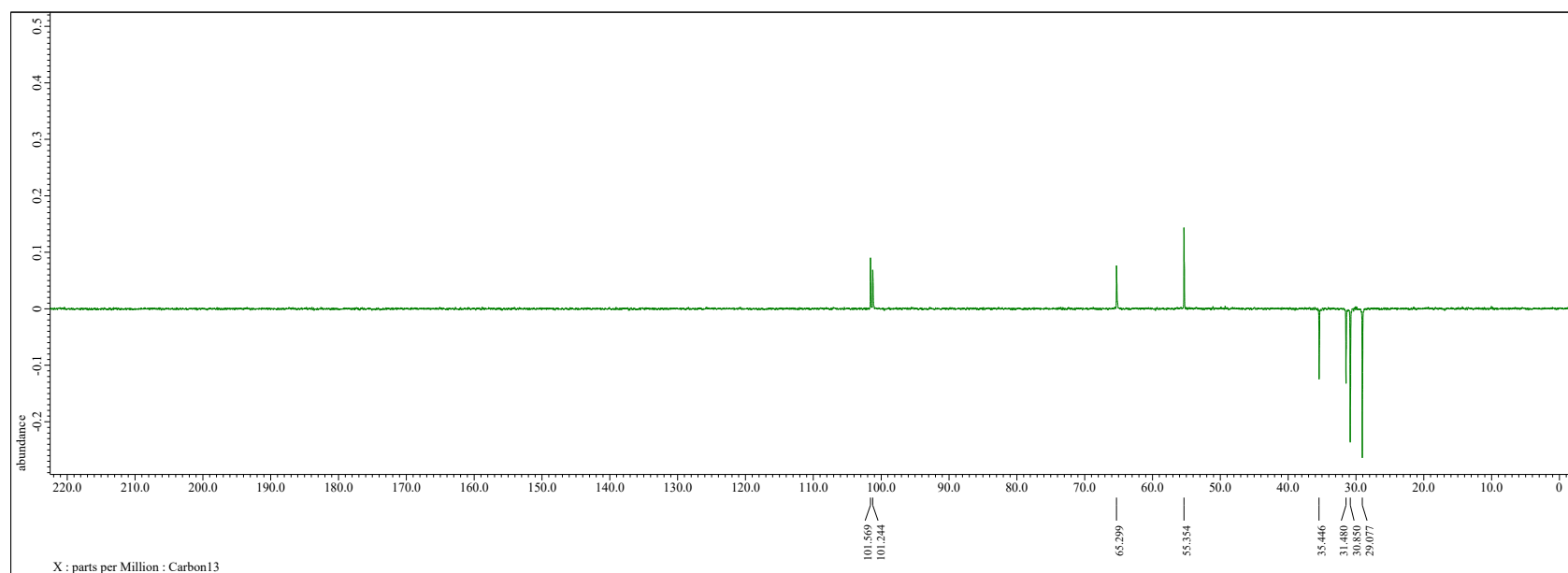


Figure S4. DEPT spectrum of **1** (Recorded in Acetone-*d*₆)

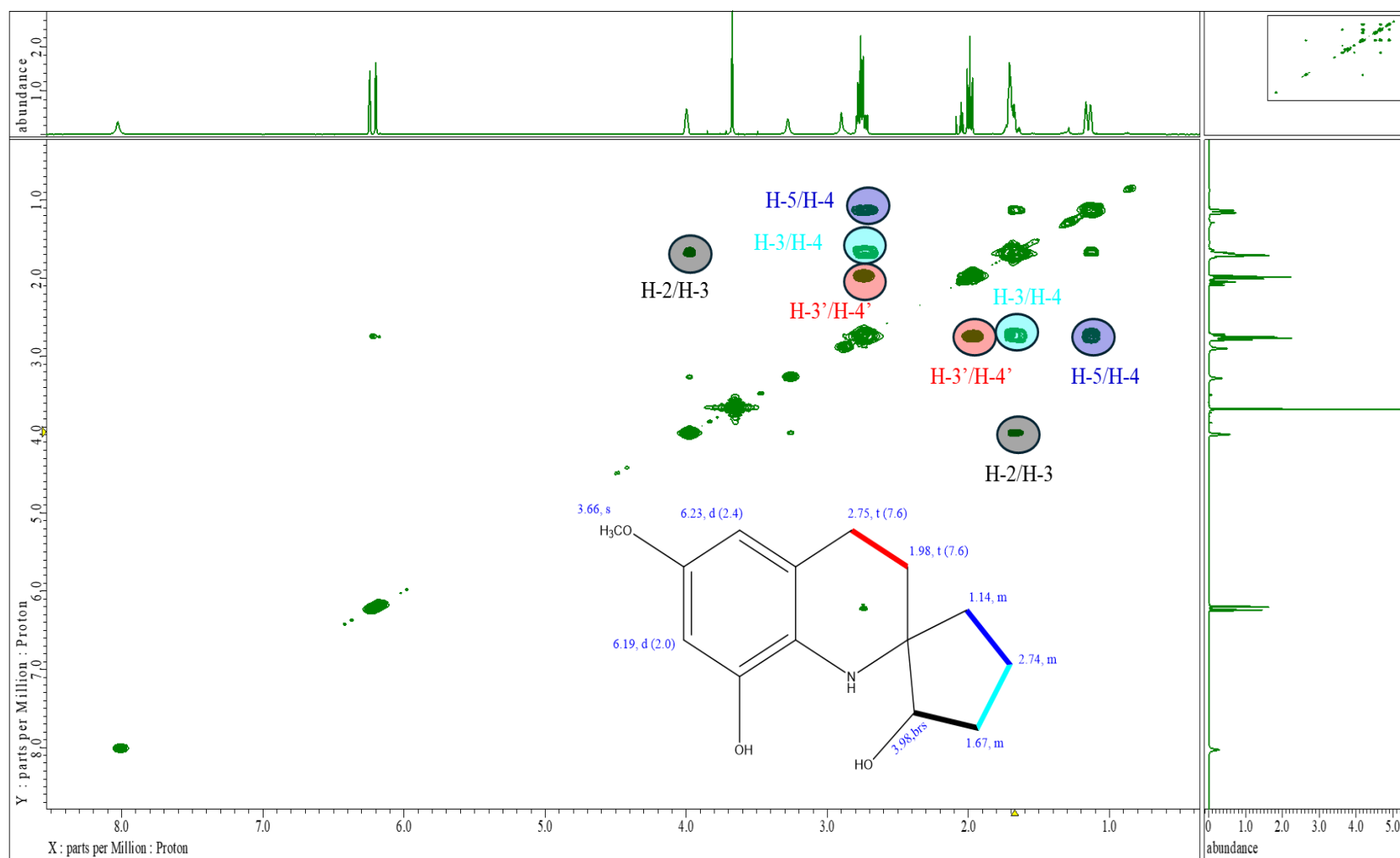


Figure S5. COSY spectrum of **1**

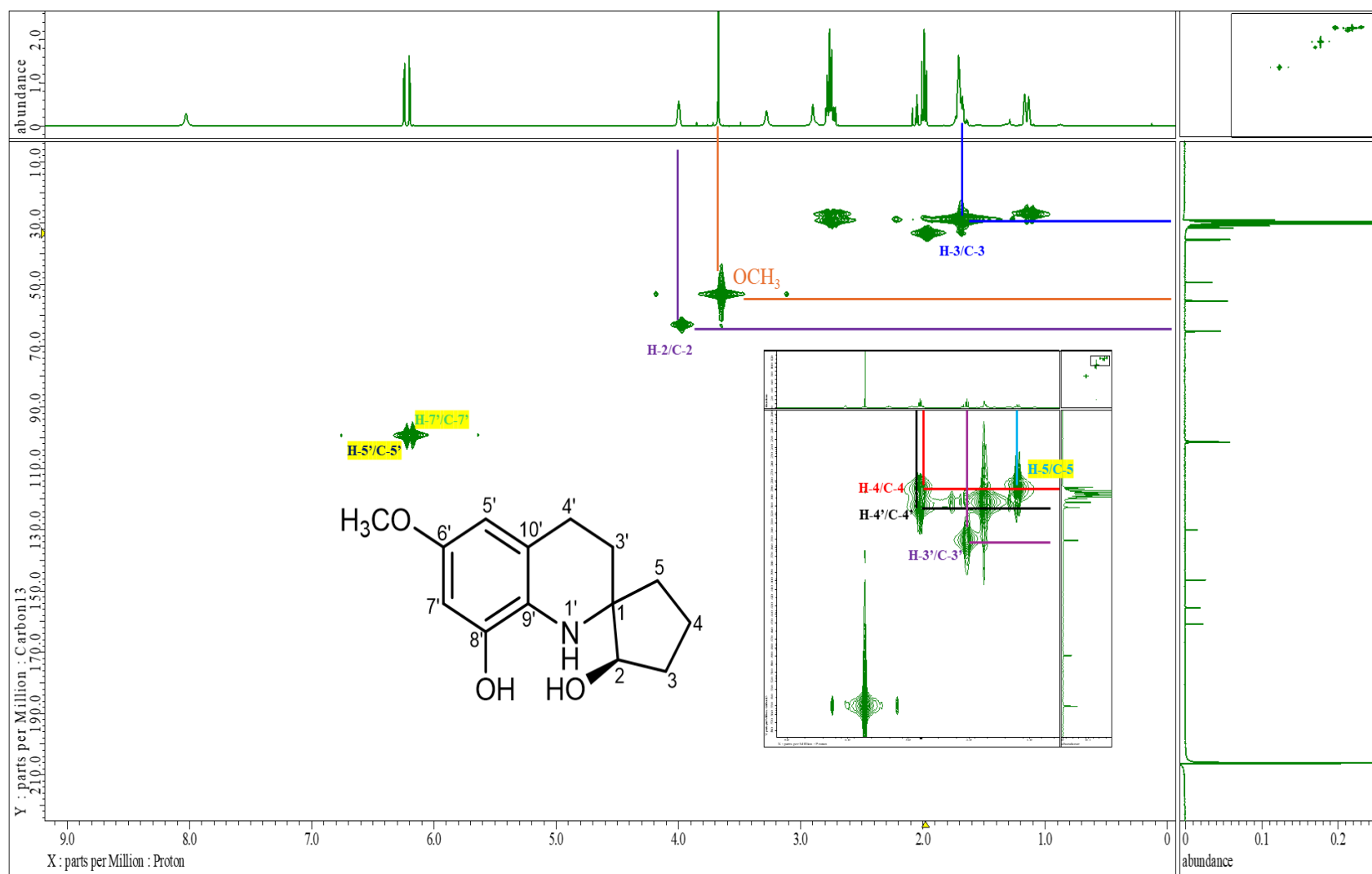


Figure S6. HMQC spectrum of **1**

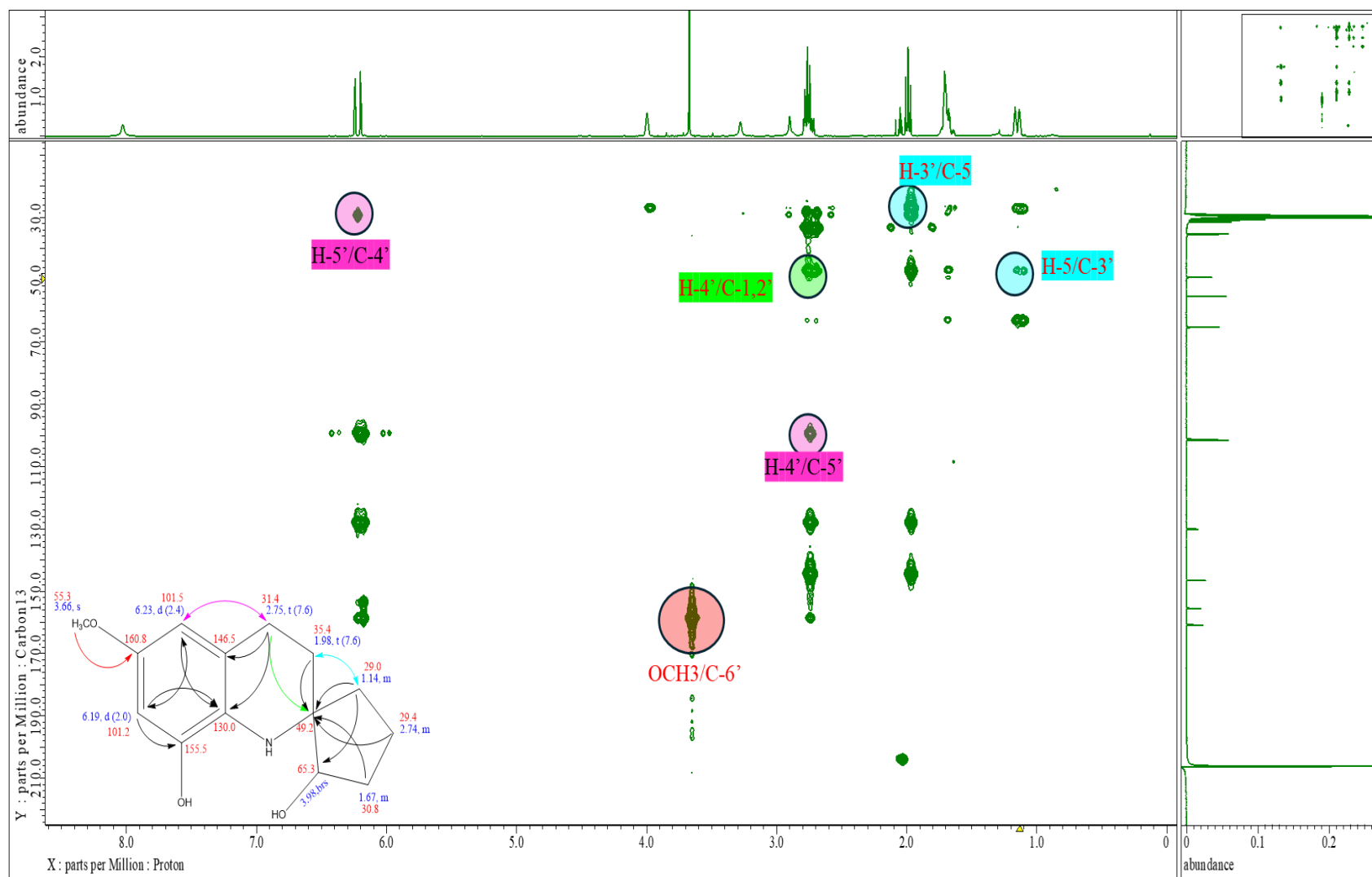


Figure S7. HMBC spectrum of **1**

scifinder-n.cas.org/search/substance/68d6413dff9c293a2684d66c/1

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View Related Results

Filter Results

Structure Match

As Drawn (0)

Substructure (0)

Similarity (130K)

Behavior

Filter by Exclude

Search Within Results

Similarity

85-89 (26)

80-84 (202)

75-79 (1,527)

70-74 (6,929)

65-69 (29K)

60-64 (88K)

Commercial Availability

Available (26)

Number of Components

1 (26)

Molecular Weight

LogP

Stereochemistry

Element

Functional Group

Aromatic Rings

Substance Class

Filtering: Similarity: 85-89 Number of Components: 1

26 Results

Sort: Molecular Formula: Ascending View: Partial

1 85 ***

2574116-40-6

C13H17NO3
3',4'-Dihydro-7'-methoxyspiro[cyclobutane-1,1'(2'H)-isoquinoline]-3,5'-diol

2 86 ***

2601915-29-9

C14H19NO3
3',4'-Dihydrospiro[cyclohexane-1,1'(2'H)-isoquinoline]-3,6',8'-triol

3 90 ***

2555123-80-1

C14H19NO3
3',4'-Dihydro-7'-methoxyspiro[cyclopentane-1,1'(2'H)-isoquinoline]-3,5'-diol

4 85 ***

2550580-31-7

C14H19NO3
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5 88 ***

2533651-04-4

C14H19NO3
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6 85 ***

2513300-77-9

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7 86 ***

2436500-92-2

C14H19NO3
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8 85 ***

2591035-09-3

C15H21NO2
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9 86 ***

1267769-67-4

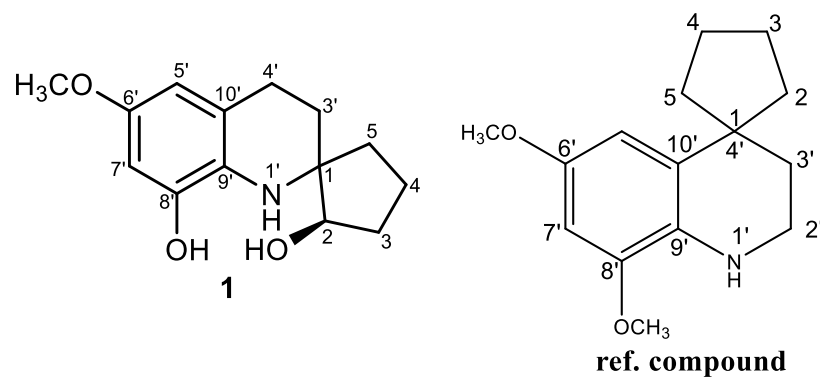
C15H21NO2
1',4'-Dihydro-5',7'-dimethoxyspiro[cyclopentane-1,3'(2'H)-isoquinoline]

Figure S8. The research results for compound 1 were obtained from Scifider database

Table 1. The comparison ^1H and ^{13}C NMR spectroscopic data of **1** and ref. compound

Position	1^a		ref. compound ^b	
	δ_{H} (J in Hz)	δ_{C}		
1	-	49.2	-	39.3
2	3.98 (1H, <i>brs</i>)	65.3	1.60 – 2.00 (m)	42.9
3	1.67 (2H, <i>m</i>)	30.8	1.60 – 2.00 (m)	25.3
4	2.73 (2H, <i>m</i>)	29.4	1.60 – 2.00 (m)	25.3
5	1.14 (2H, <i>m</i>)	29.0	1.60 – 2.00 (m)	42.9
1'	-	-	4.04 (1H, <i>brs</i>)	-
2'	-	-	3.25 (2H, <i>t</i> , 5.6)	36.0
3'	1.98 (2H, <i>t</i> , 7.6)	35.4	1.60 – 2.00 (m)	43.9
4'	2.75 (2H, <i>t</i> , 7.6)	31.4	-	-
5'	6.23 (1H, <i>d</i> , 2.2)	101.5	6.38 (1H, <i>d</i> , 2.4)	102.8
6'	-	160.8	-	151.4
7'	6.19 (1H, <i>d</i> , 2.2)	101.2	6.29 (1H, <i>d</i> , 2.4)	96.2
8'	-	155.5	-	147.0
9'	-	130.0	-	128.5
10'	-	146.5	-	130.7
OCH ₃	3.66 (3H, <i>s</i>)	55.3	3.75 (3H, <i>s</i>)	55.8
OCH ₃	-	-	3.80 (3H, <i>s</i>)	55.4

a: recorded in acetone-*d*₆; b: recorded in CDCl₃; ref.compound: (6',8'-Dimethoxy-2',3'-dihydro-1'H-spiro[cyclopentane-1,4-quinolin] [1]



2. Spectroscopic data for compound 2

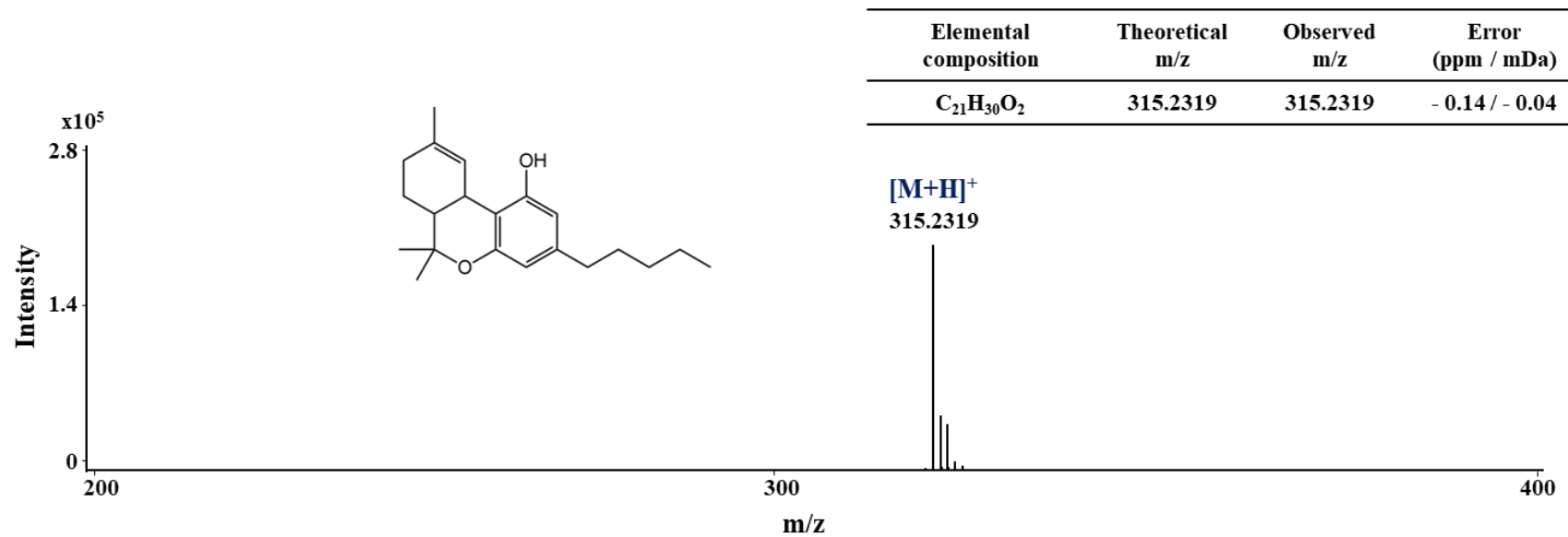


Figure S9. MS spectrum of 2

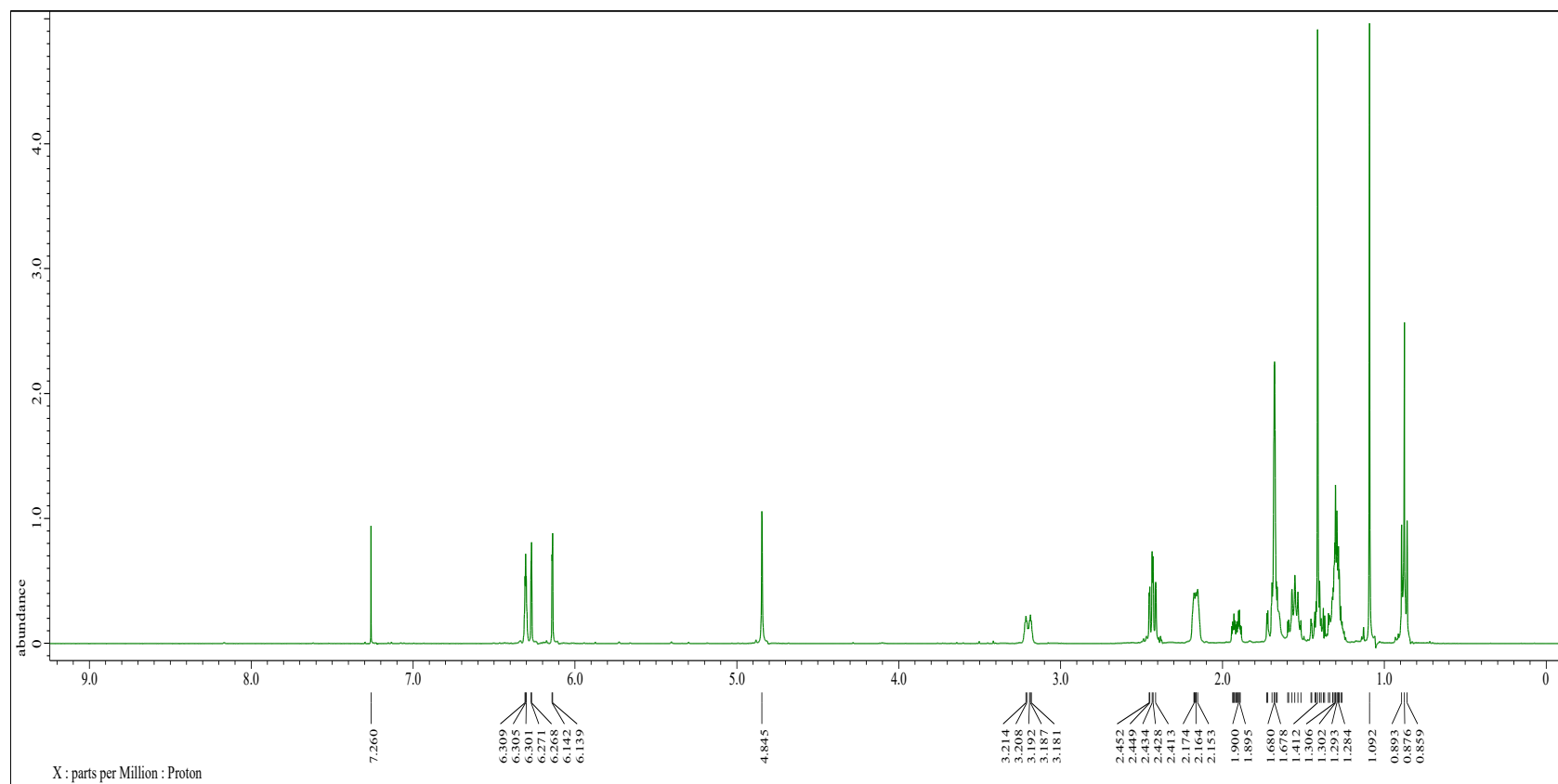


Figure S10. ^1H NMR spectrum of **2** (Recorded in CDCl_3)

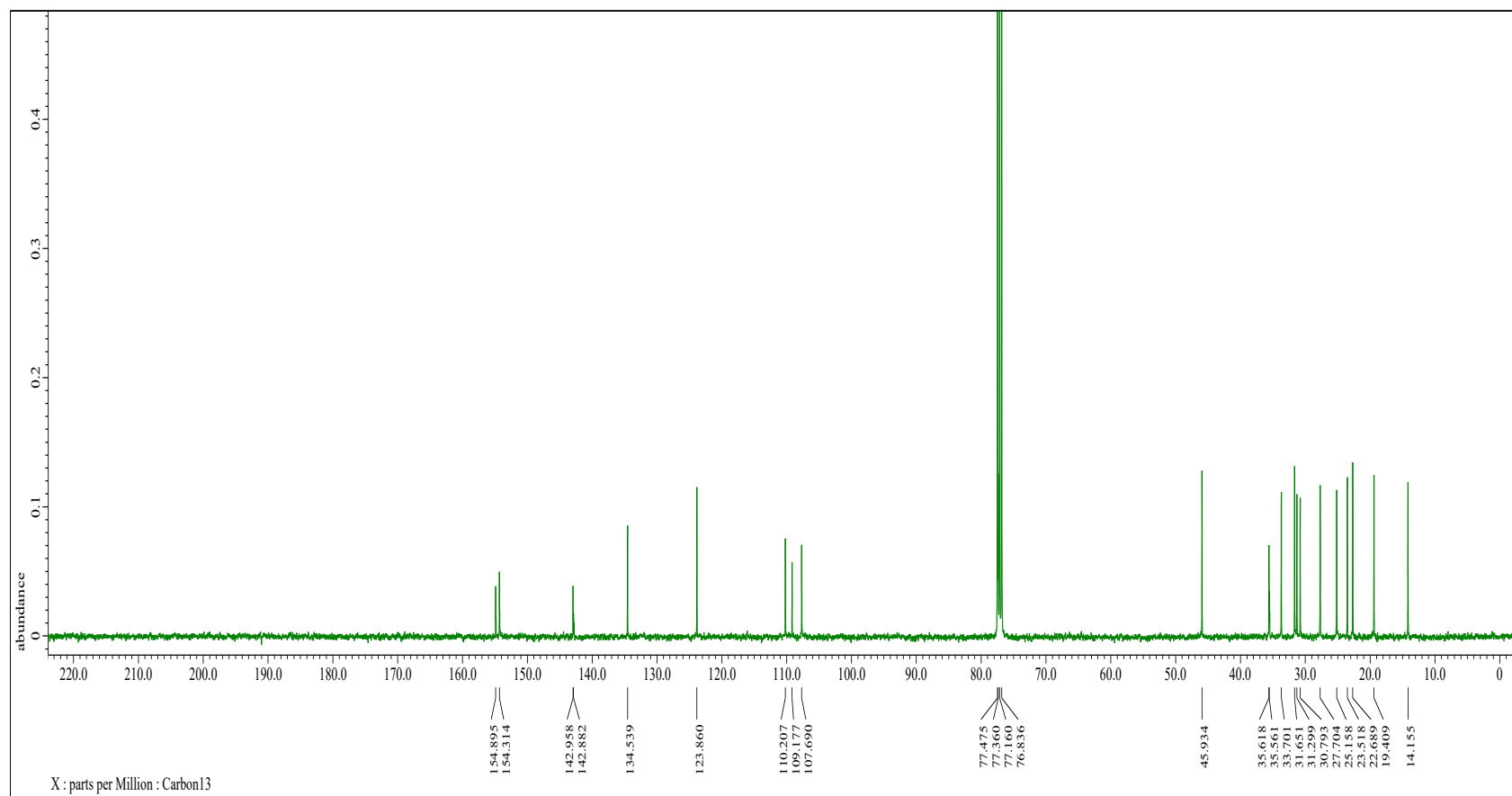


Figure S11. ^{13}C NMR spectrum of **2** (Recorded in CDCl_3)

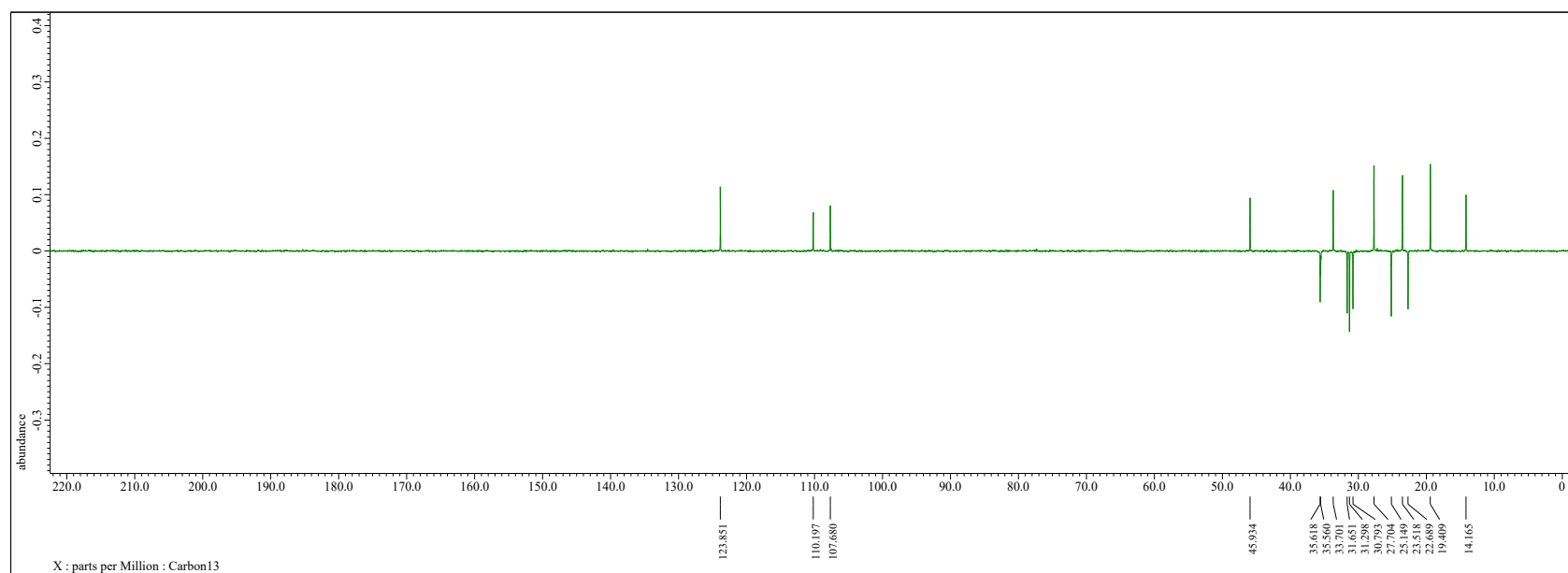


Figure S12. DEPT spectrum of **2** (Recorded in CDCl₃)

3. Spectroscopic data for compound 3

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
C ₂₂ H ₃₂ O ₄	361.2373	361.2367	1.76 / 0.64

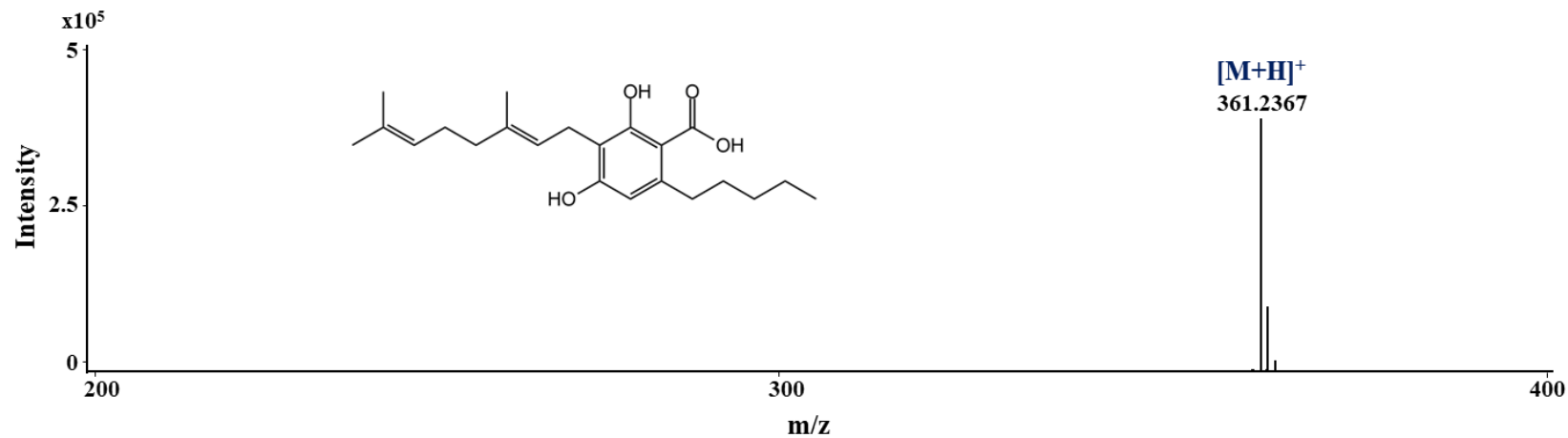


Figure S13. MS spectrum of 3

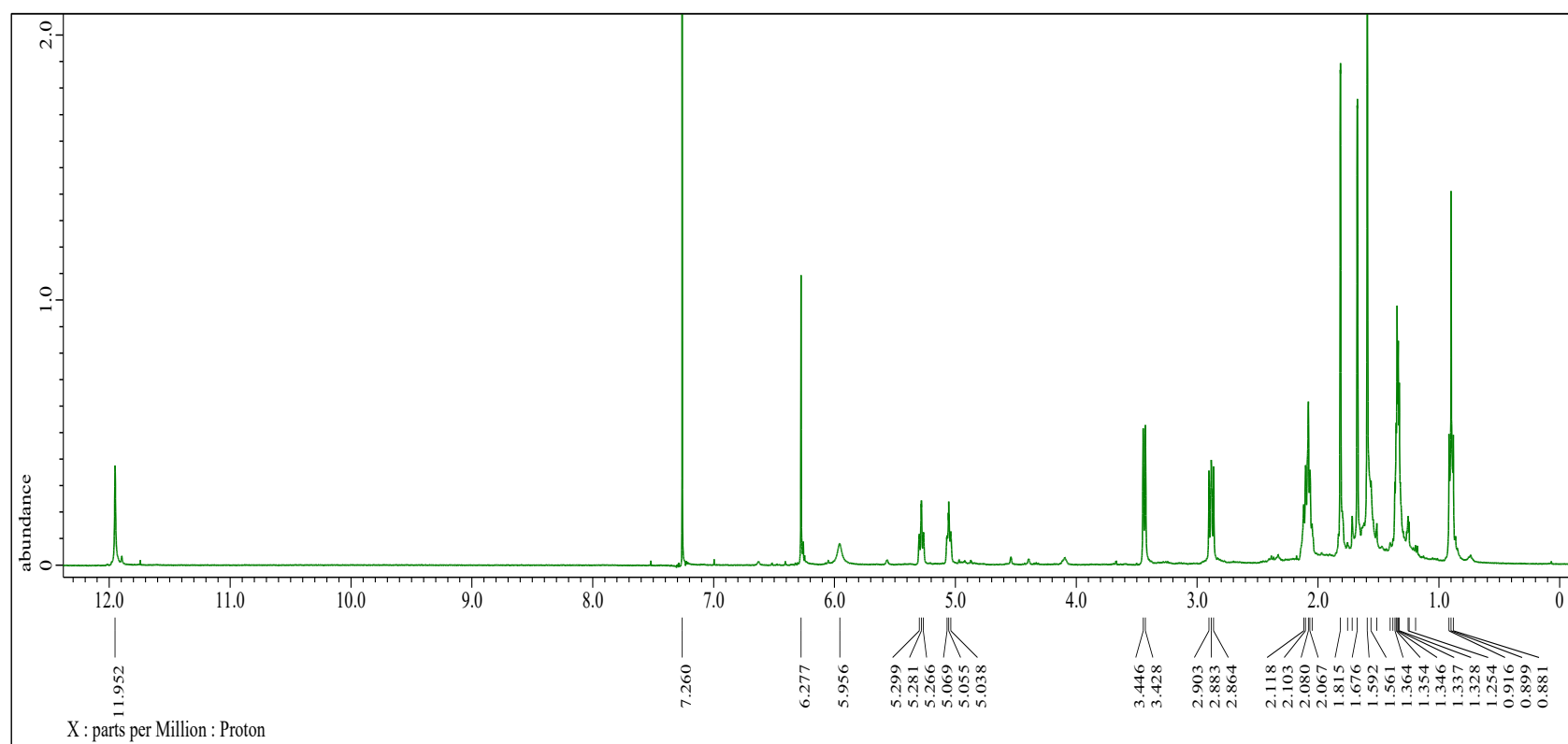


Figure S14. ^1H NMR spectrum of **3** (Recorded in CDCl_3)

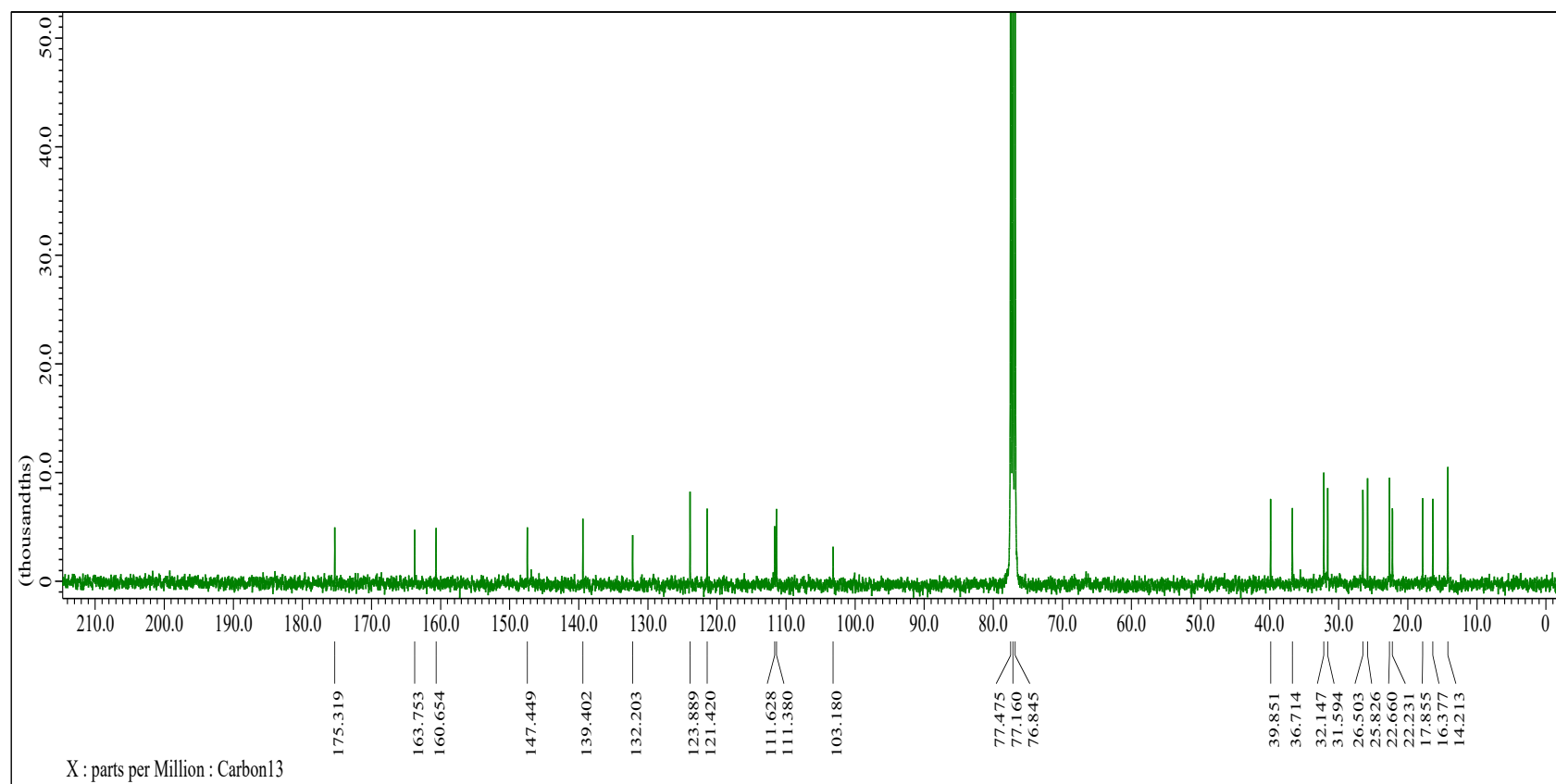


Figure S15. ¹³C NMR spectrum of **3** (Recorded in CDCl₃)

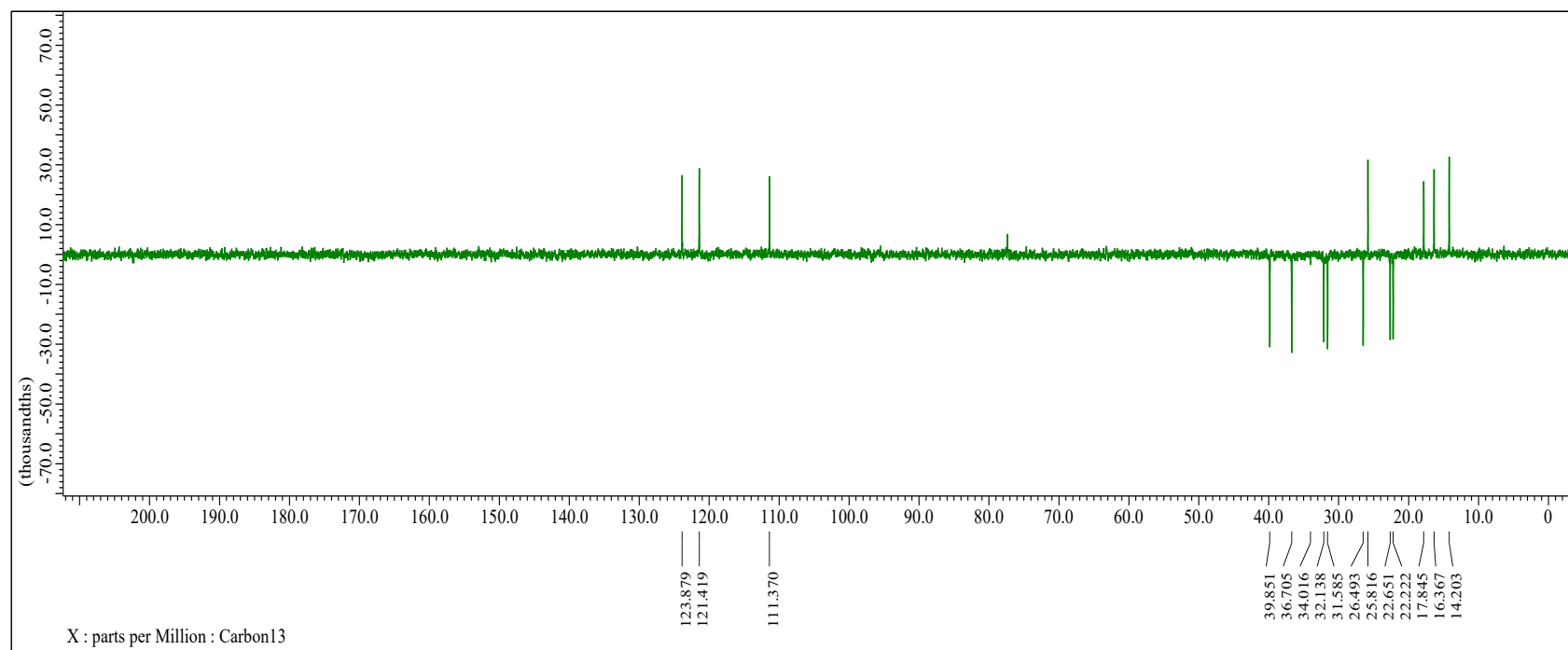


Figure S16. DEPT spectrum of **3**

4. Spectroscopic data for compound 4

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
C ₂₁ H ₃₀ O ₂	315.2319	315.2316	0.81 / 0.26

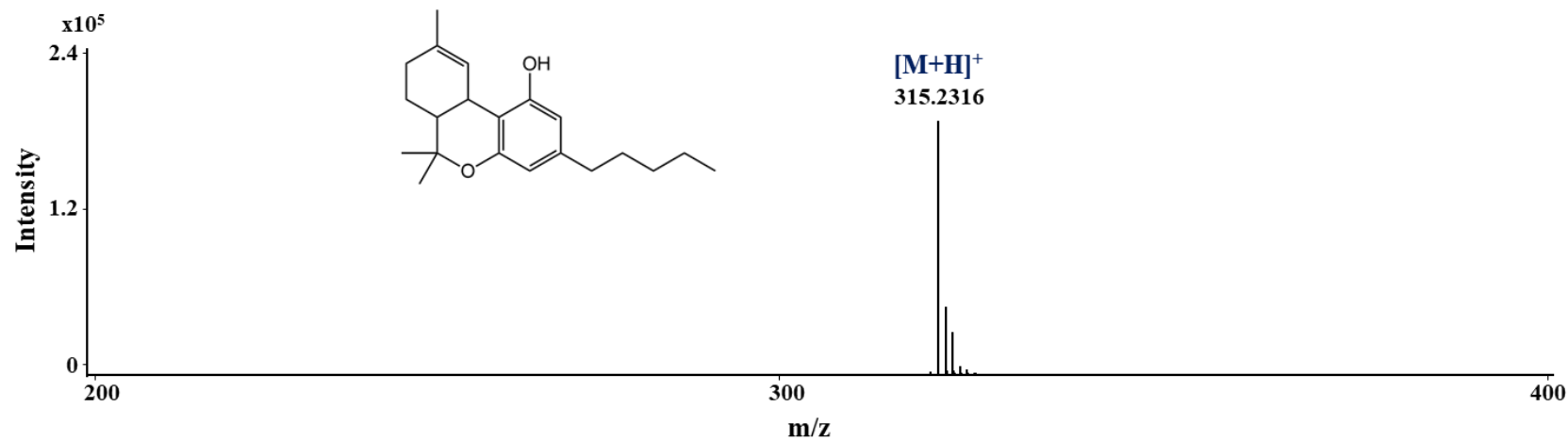


Figure S17. MS spectrum of **4**

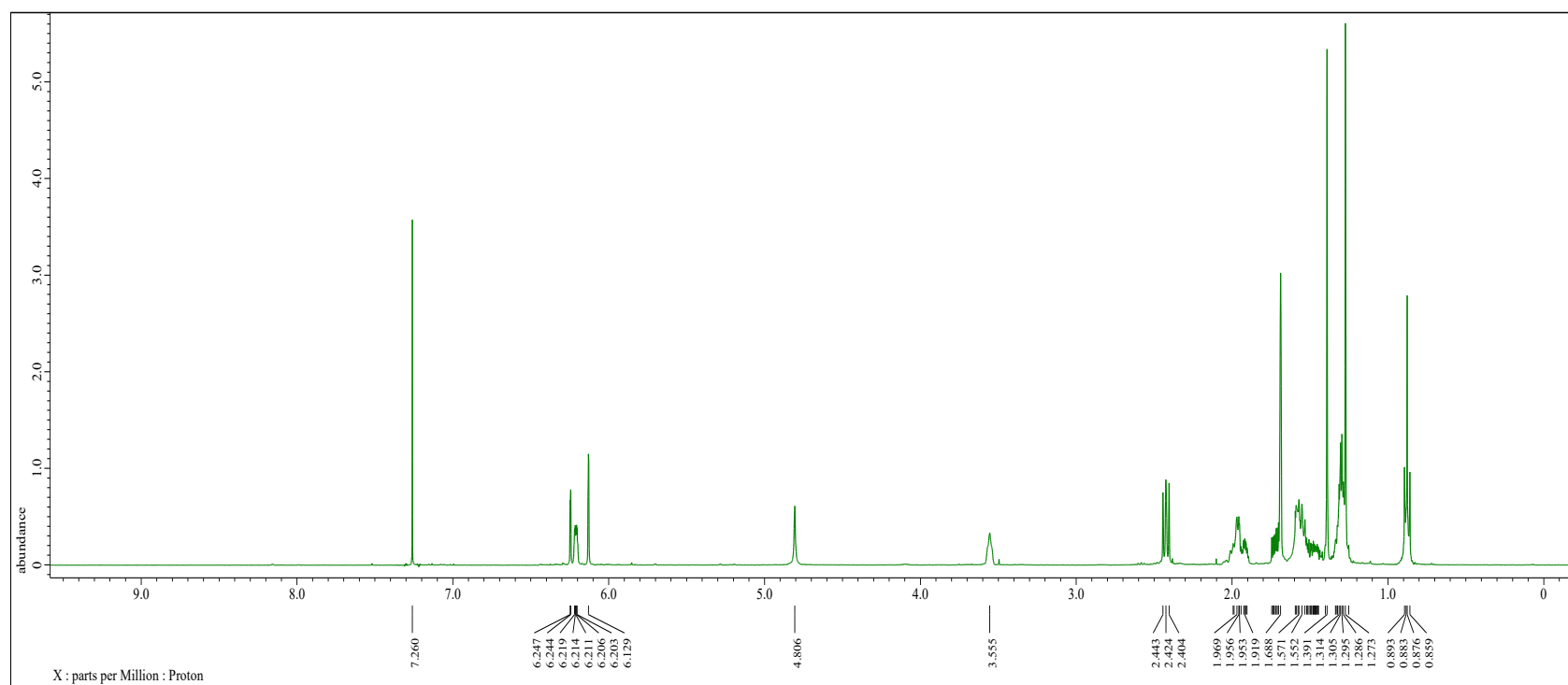


Figure S18. ^1H NMR spectrum of **4** (Recorded in CDCl_3)

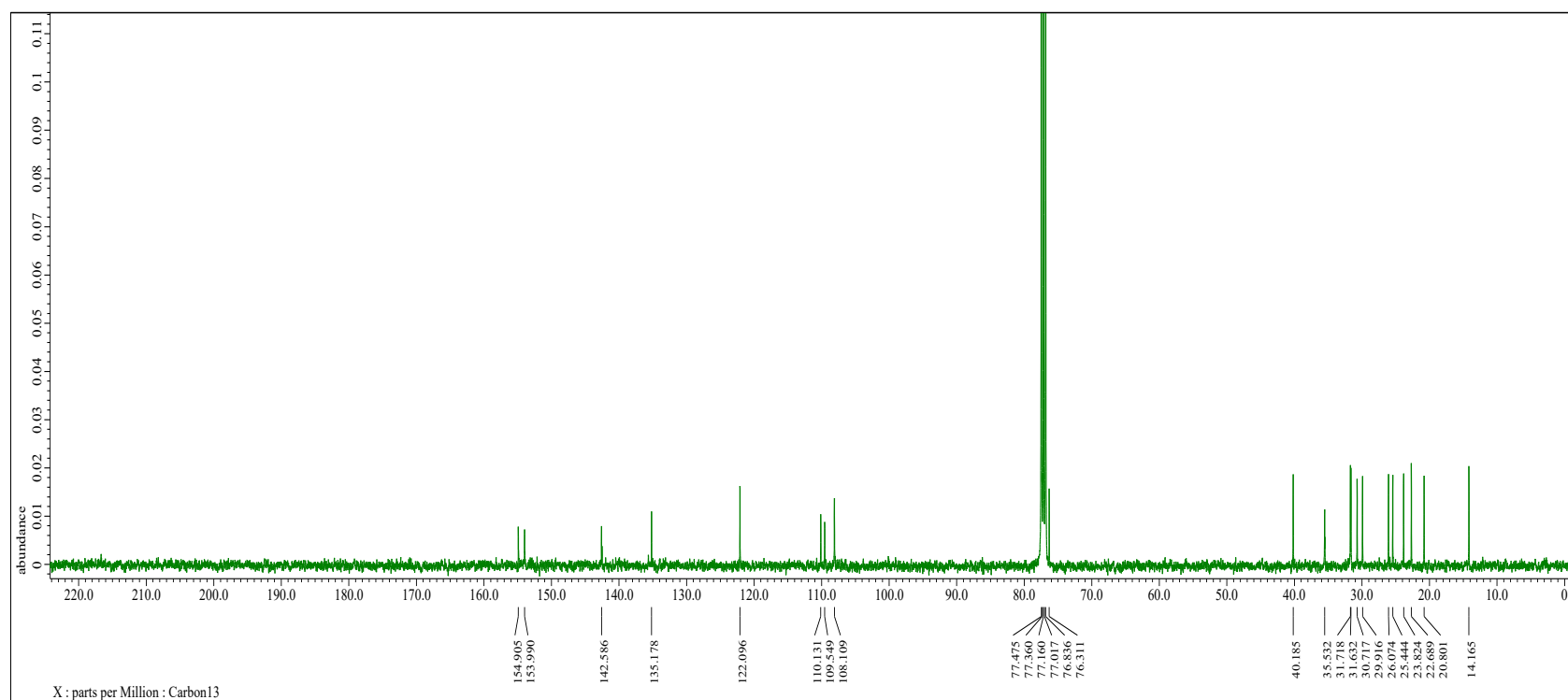


Figure S19. ¹³C NMR spectrum of **4** (Recorded in CDCl₃)

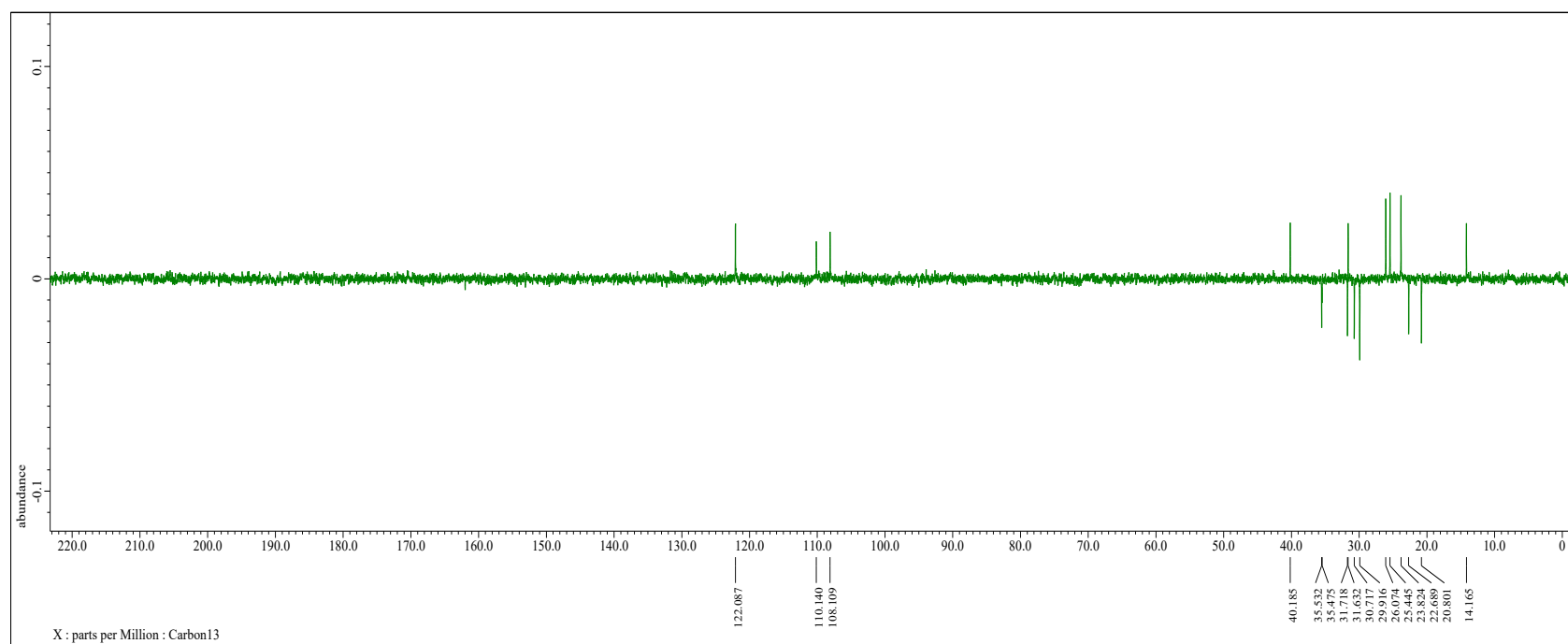


Figure S20. DEPT spectrum of **4**

5. Spectroscopic data for compound **5**

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
C ₁₅ H ₂₆ O	223.2056	223.2053	1.53 / 0.34

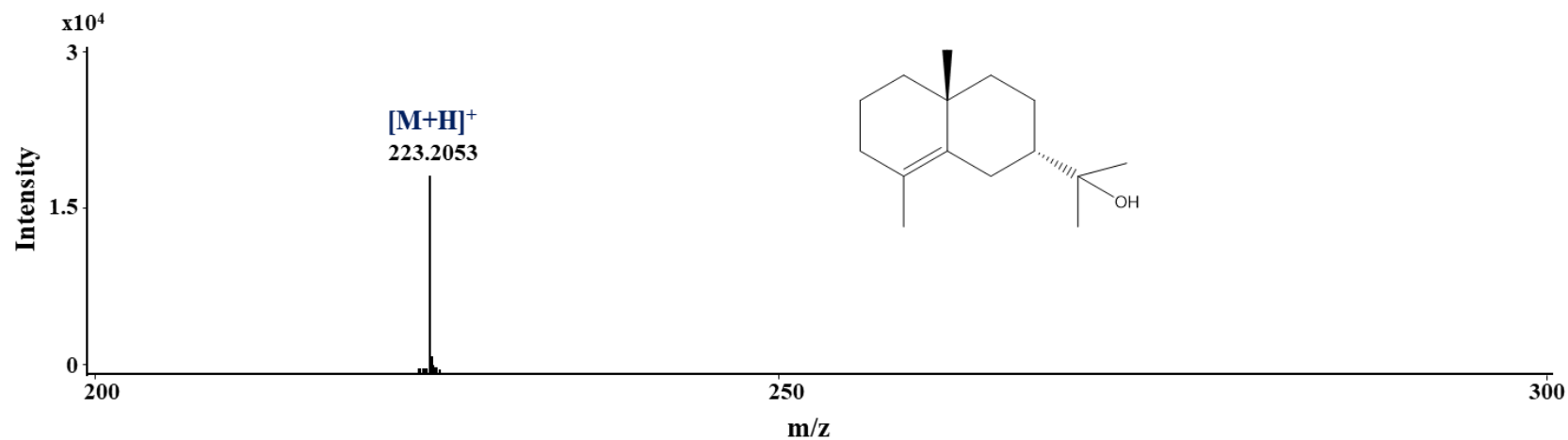


Figure S21. MS spectrum of **5**

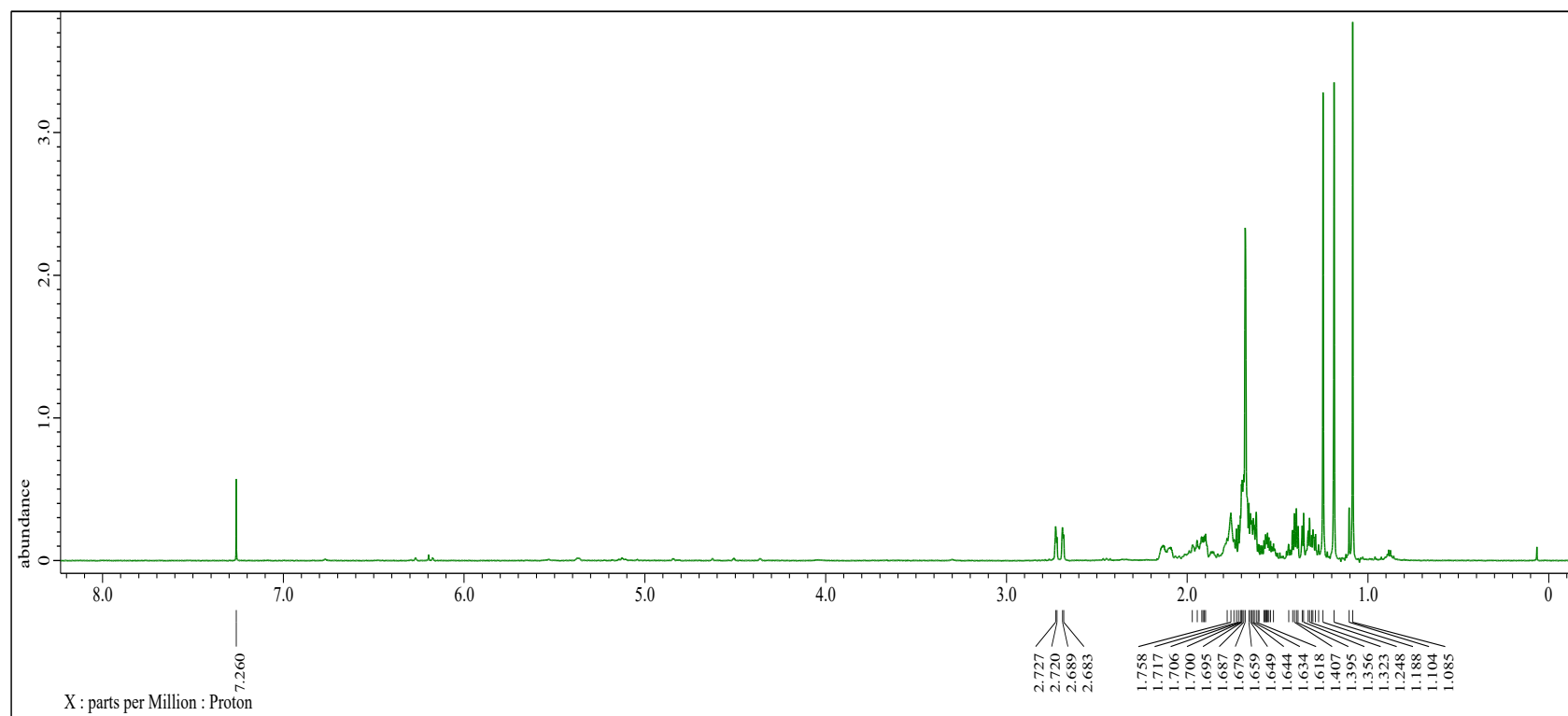


Figure S22. ^1H NMR spectrum of **5** (Recorded in CDCl_3)

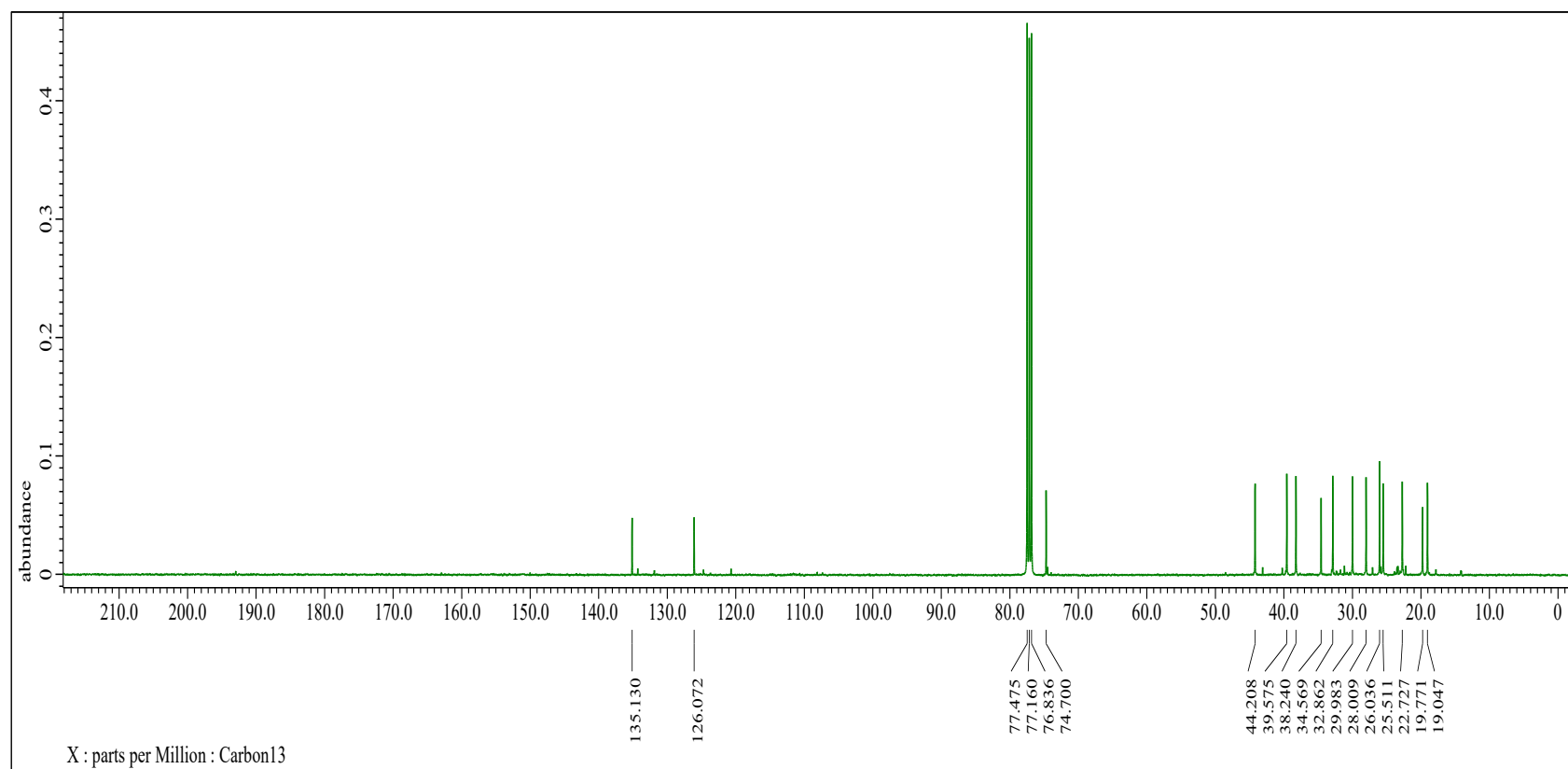


Figure S23. ¹³C NMR spectrum of **5** (Recorded in CDCl₃)

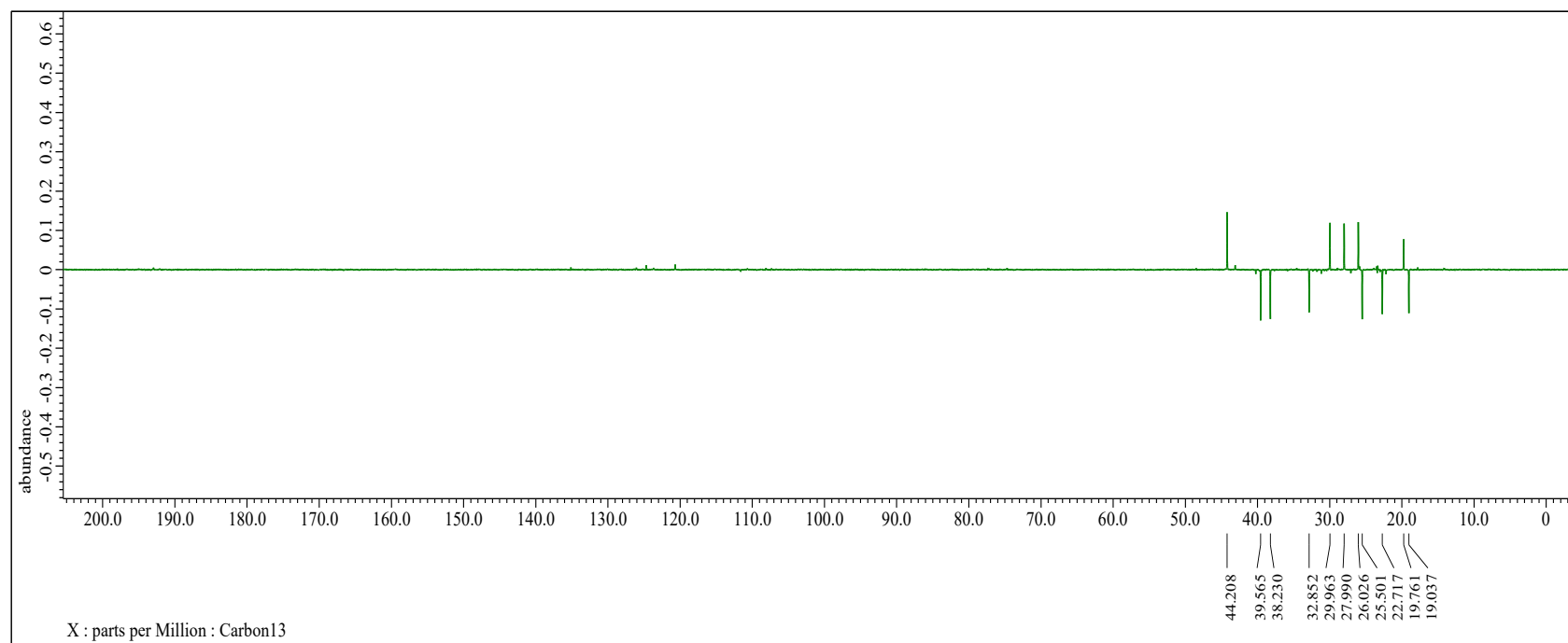


Figure S24. DEPT spectrum of **5** (Recorded in CDCl_3)

6. Spectroscopic data for compound 6

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
C ₁₅ H ₂₆ O	223.2056	223.2044	5.56 / 1.24

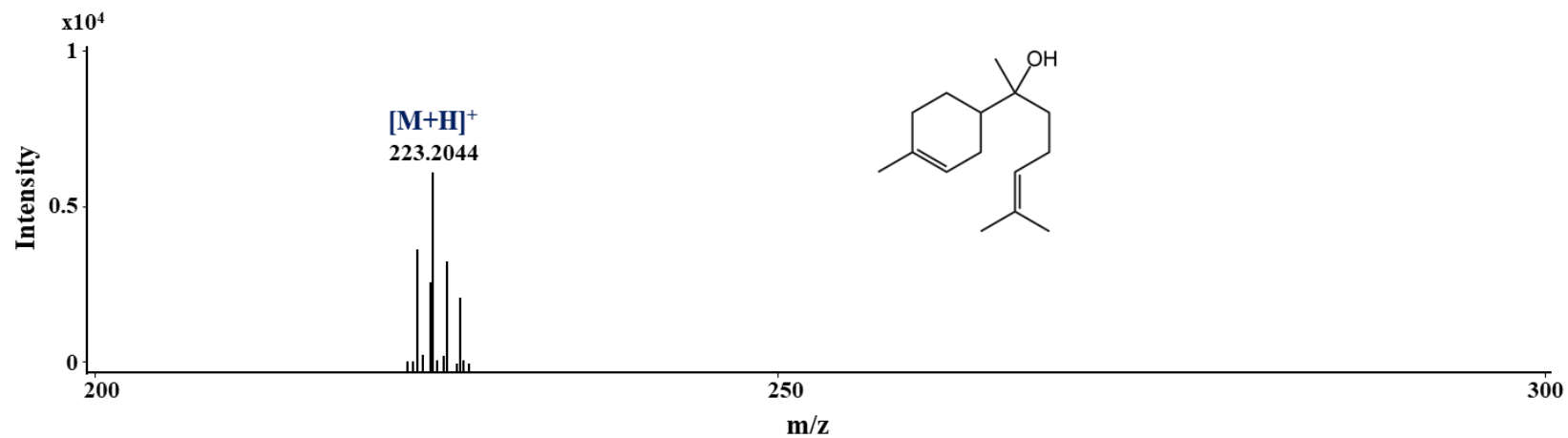


Figure S25. MS spectrum of **6**

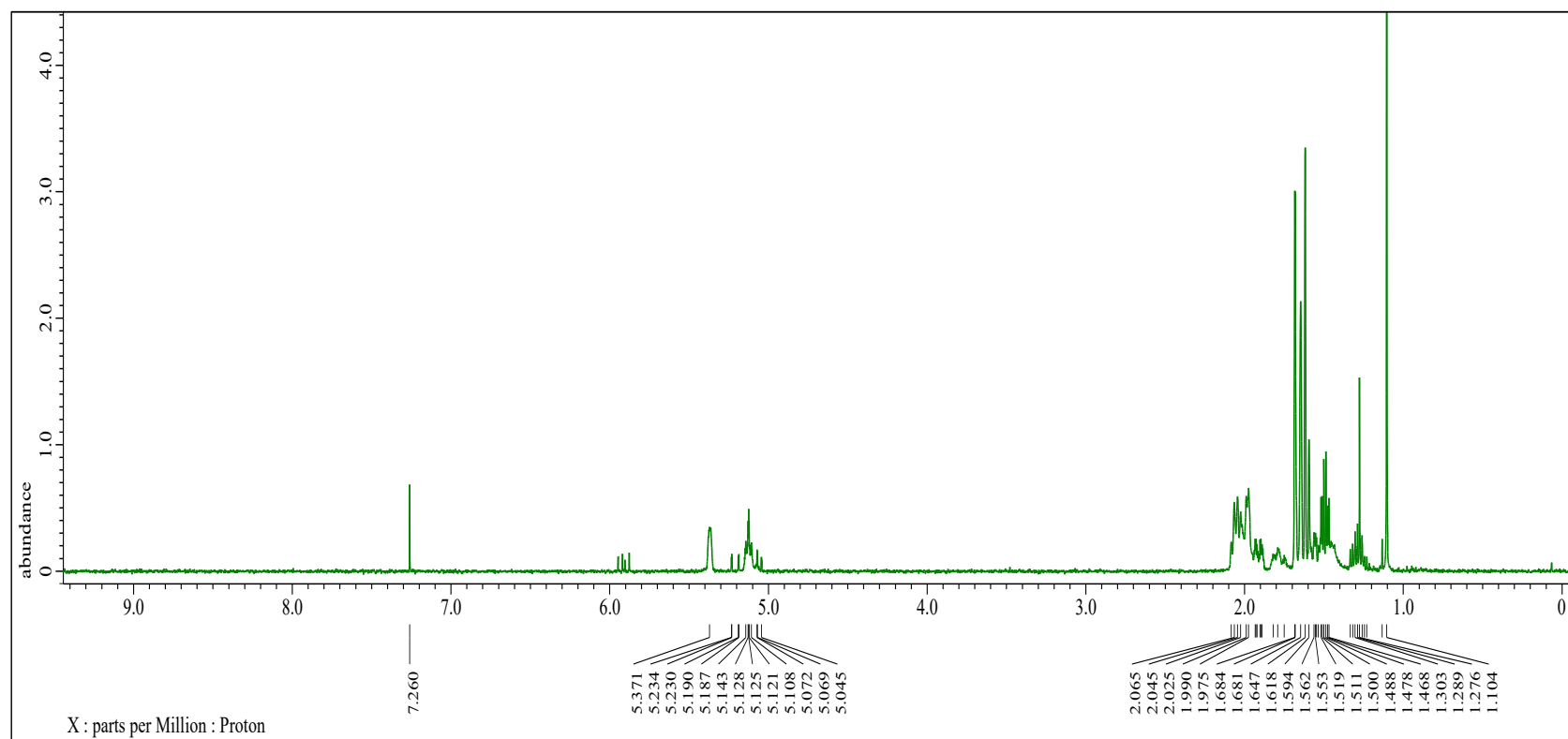


Figure S26. ^1H NMR spectrum of **6** (Recorded in CDCl_3)

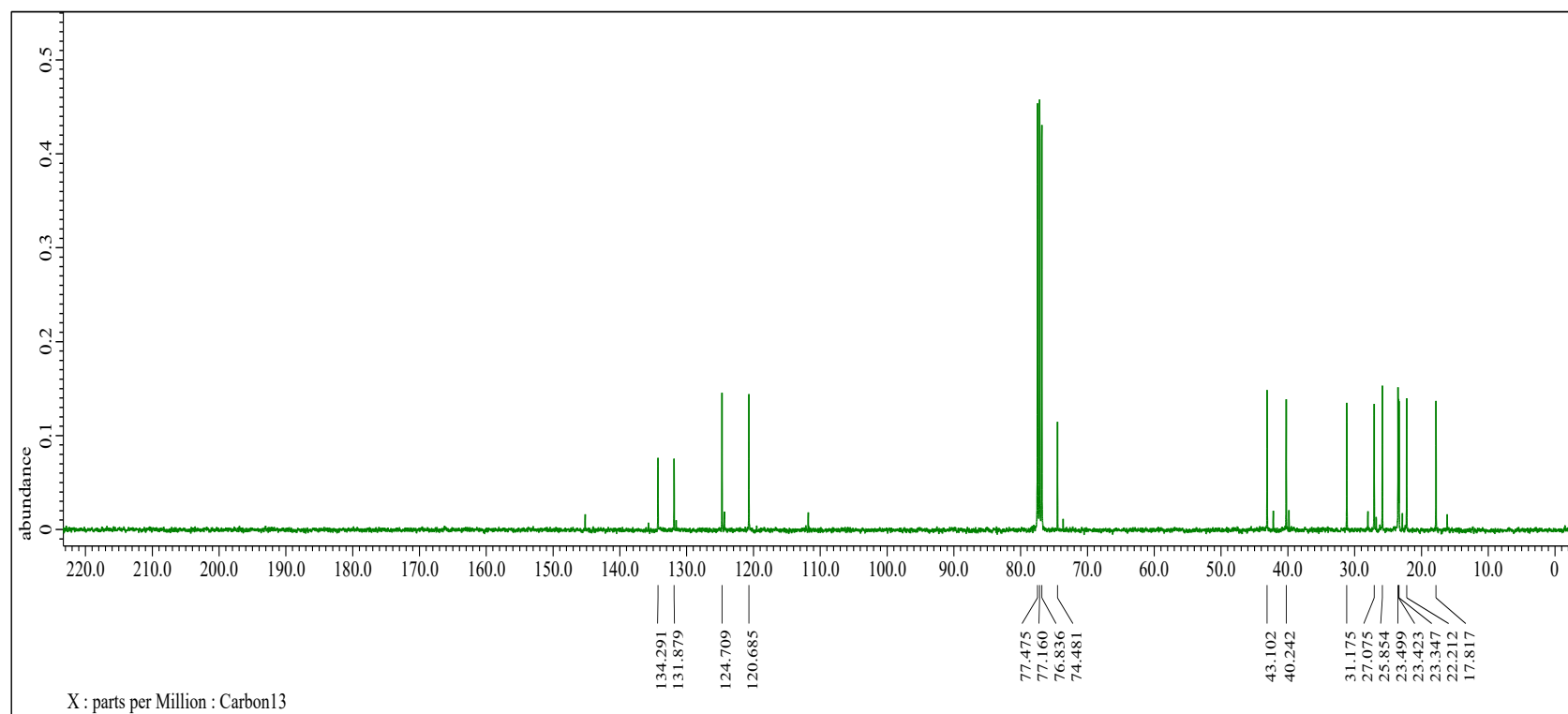


Figure S27. ^{13}C NMR spectrum of **6**

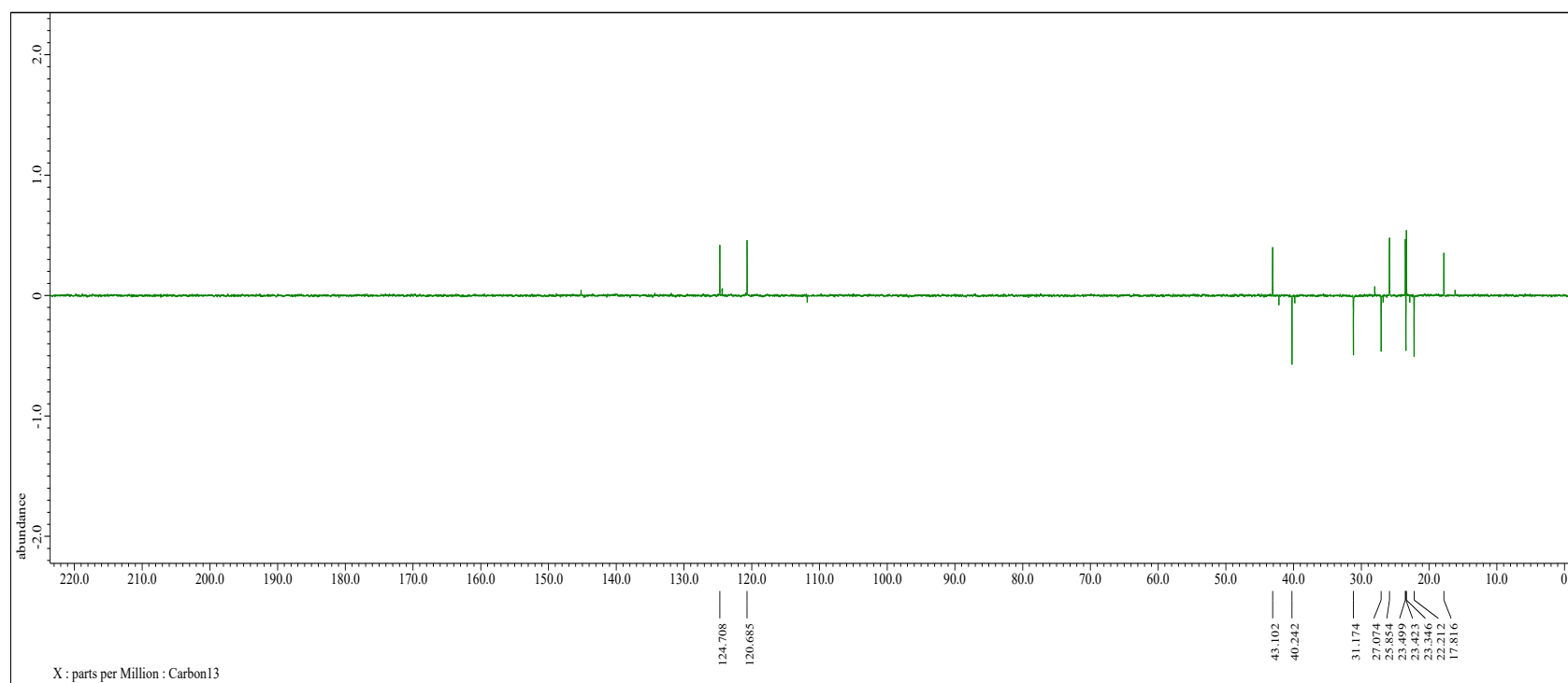


Figure S28. DEPT spectrum of **6**

7. Spectroscopic data for compound 7

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
C ₁₅ H ₂₆ O	223.2056	223.2062	-2.5 / -0.56

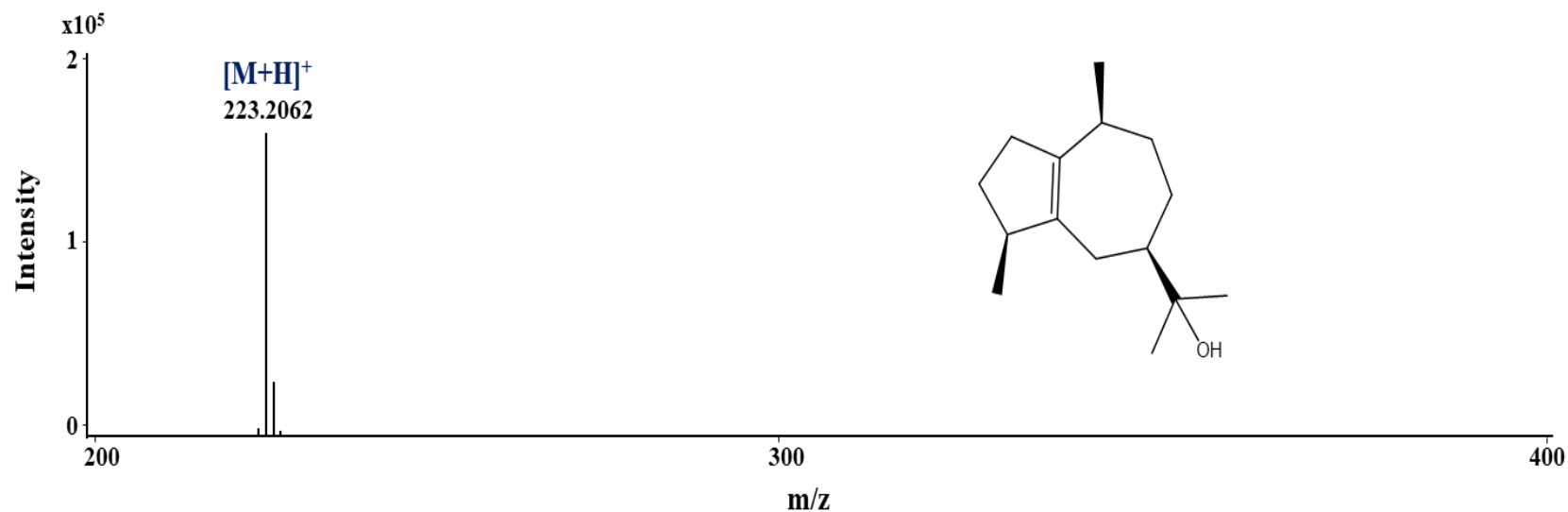


Figure S29. MS spectrum of **7**

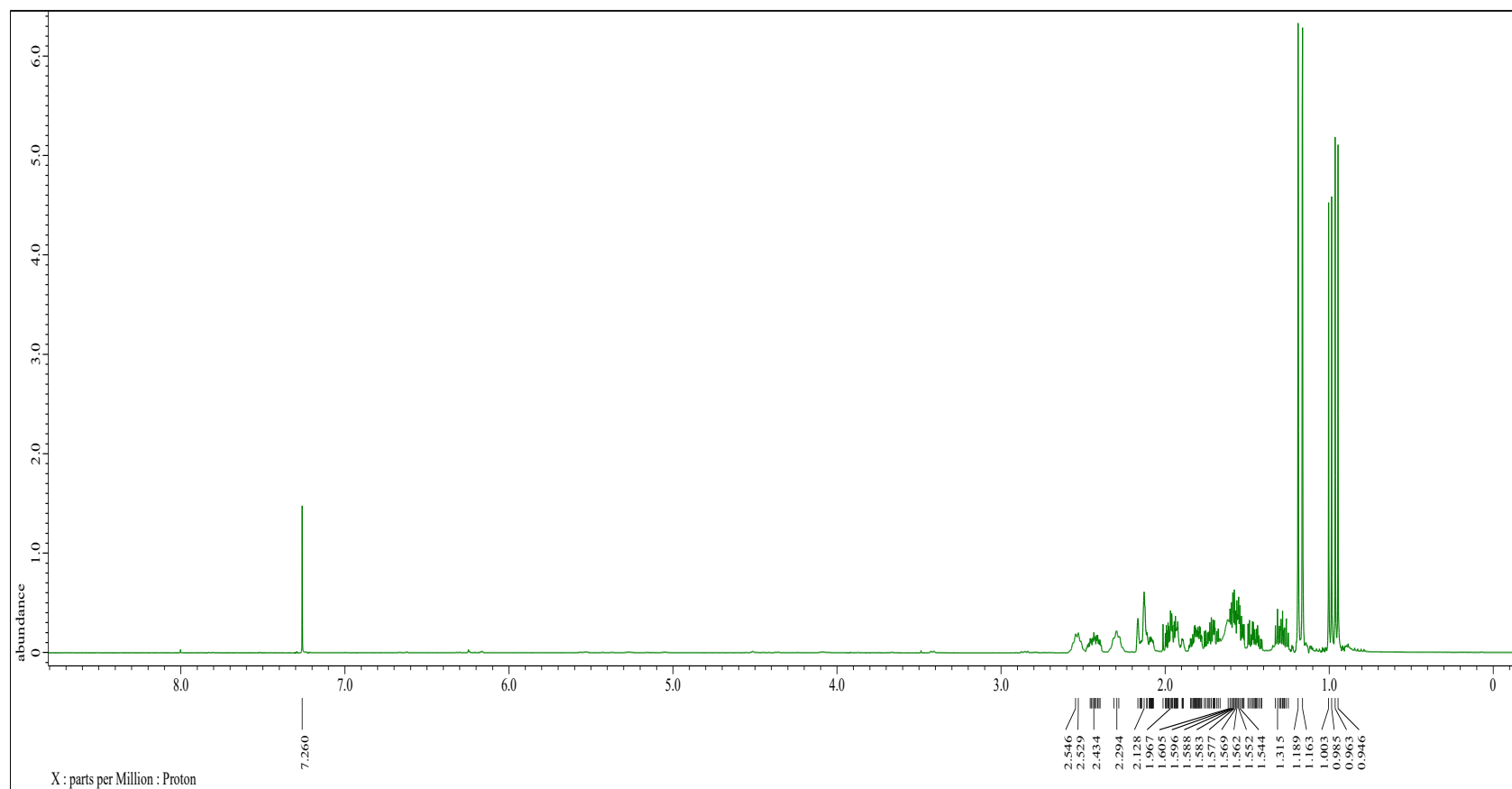


Figure S30. ^1H NMR spectrum of **7** (Recorded in CDCl_3)

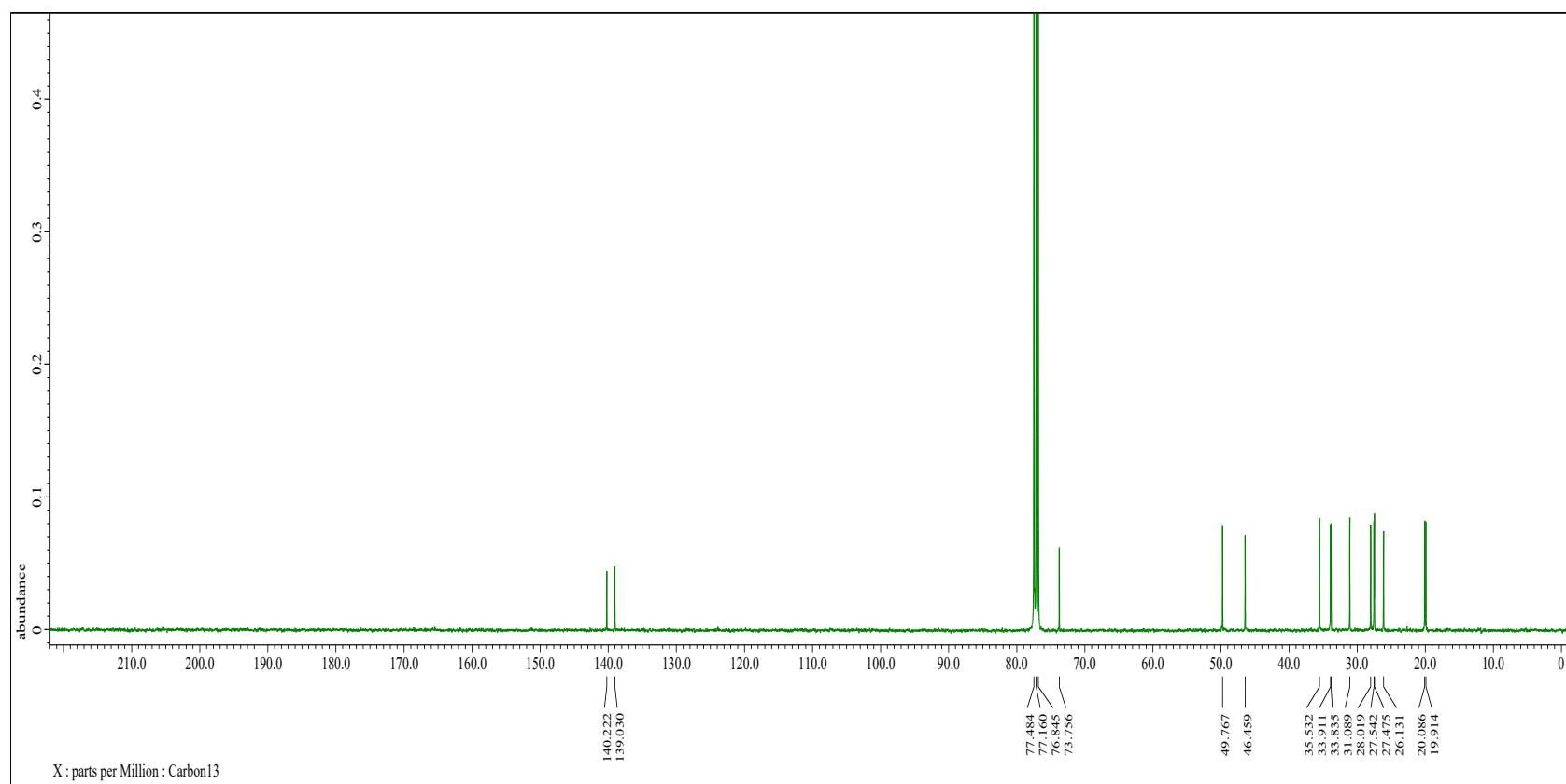


Figure S31. ^{13}C NMR spectrum of **7** (Recorded in CDCl_3)

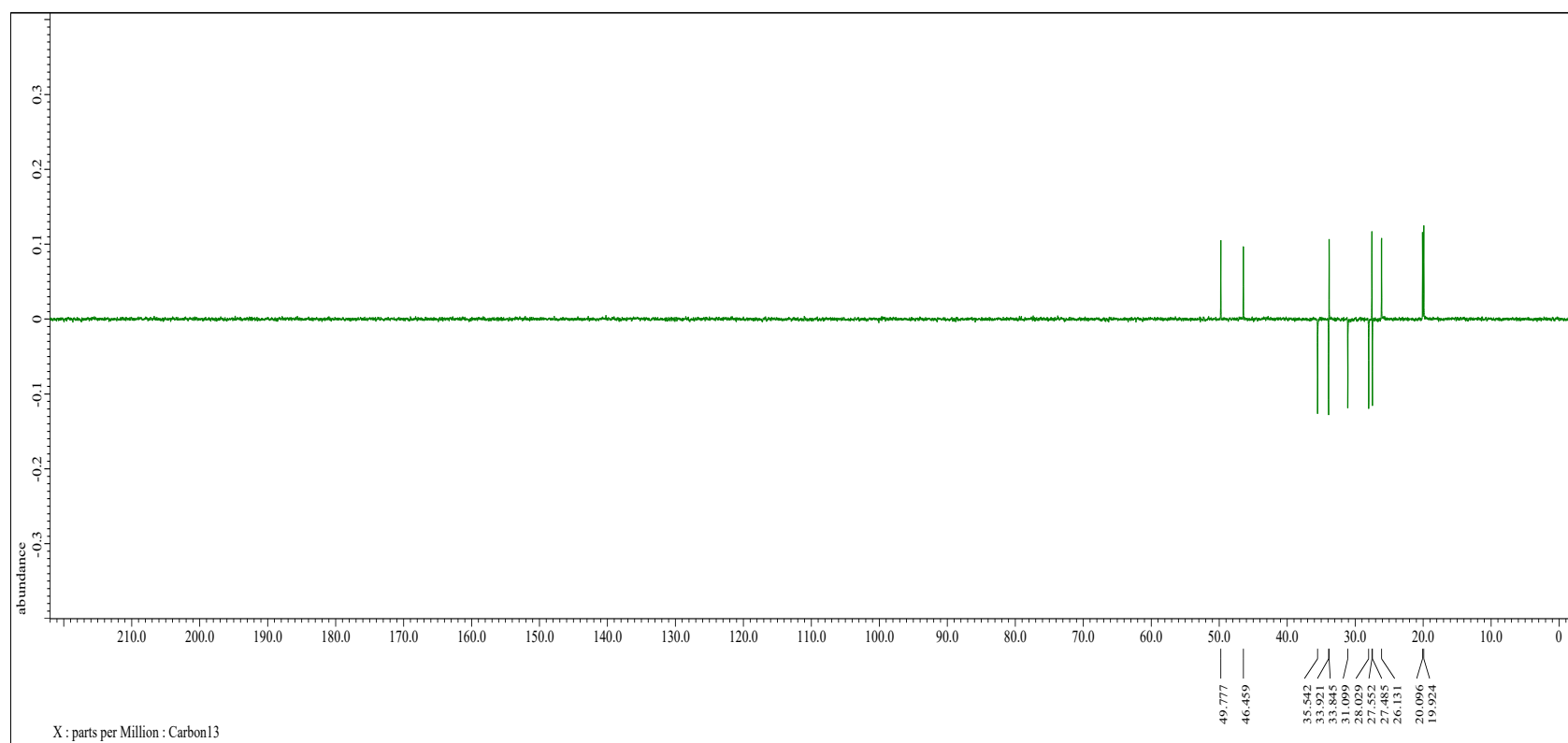


Figure S32. DEPT spectrum of **7** (Recorded in CDCl_3)

8. Spectroscopic data for compound 8

Elemental composition	Theoretical m/z	Observed m/z	Error (ppm / mDa)
C ₁₅ H ₂₆ O	223.2056	233.2047	4.22 / 0.94

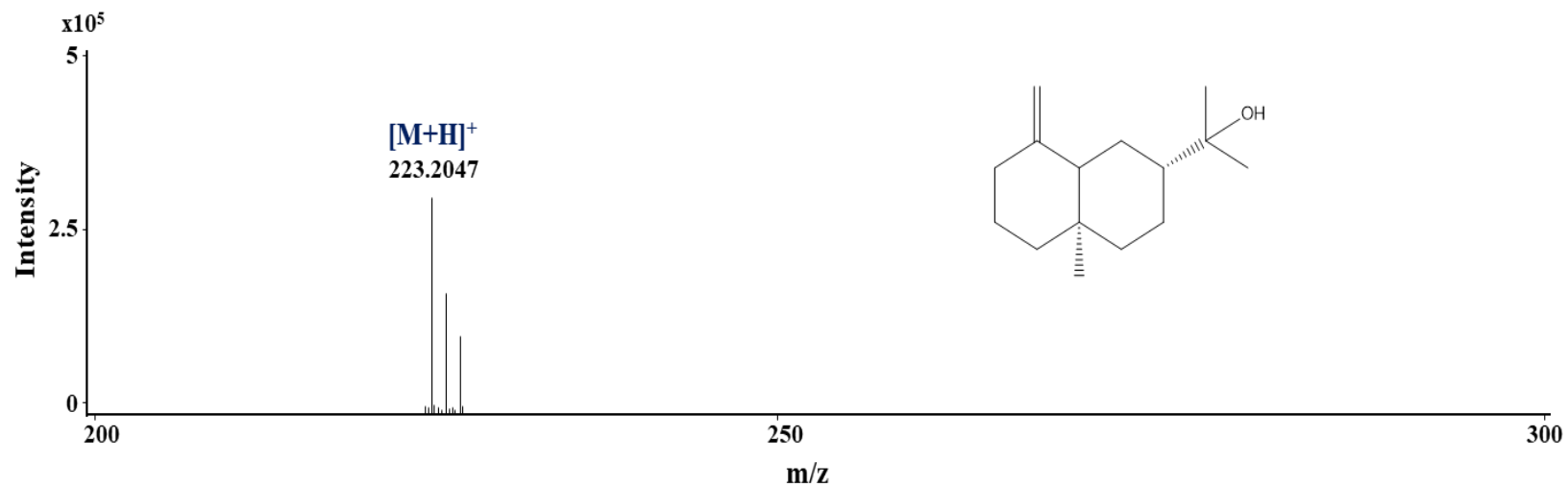


Figure S33. MS spectrum of **8**

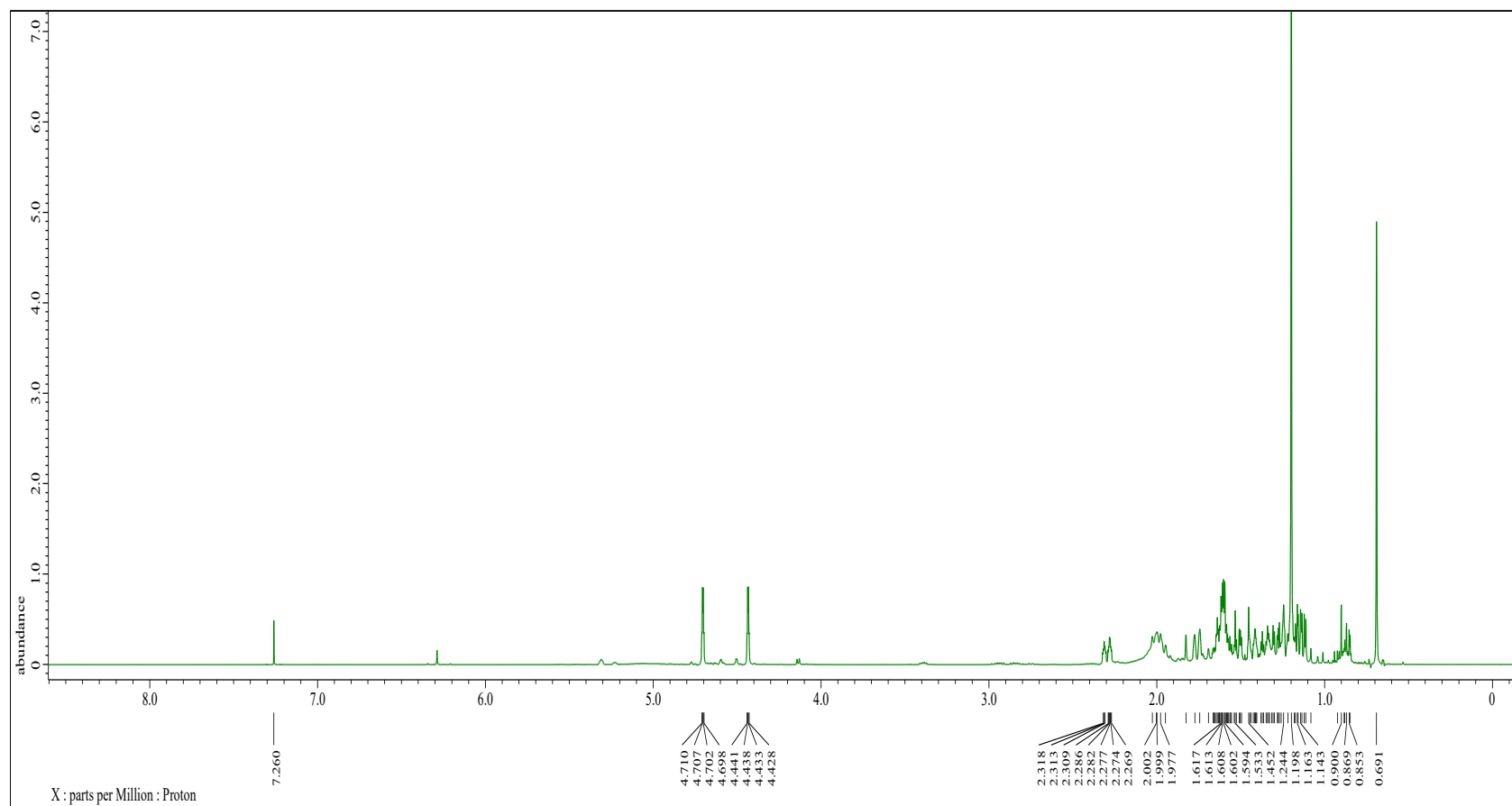


Figure S34. ^{13}C NMR spectrum of **8** (Recorded in CDCl_3)

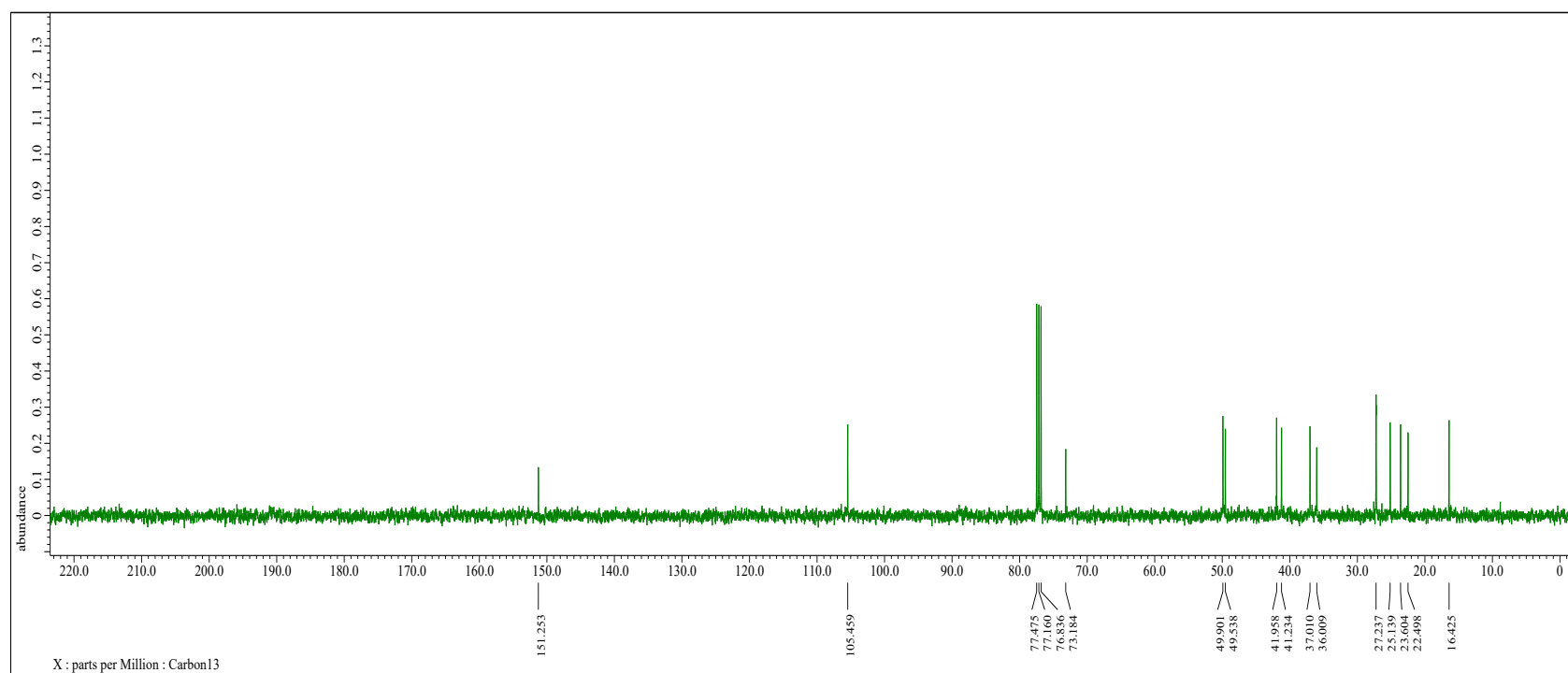


Figure S35. ¹³C NMR spectrum of **9** (Recorded in CDCl₃)

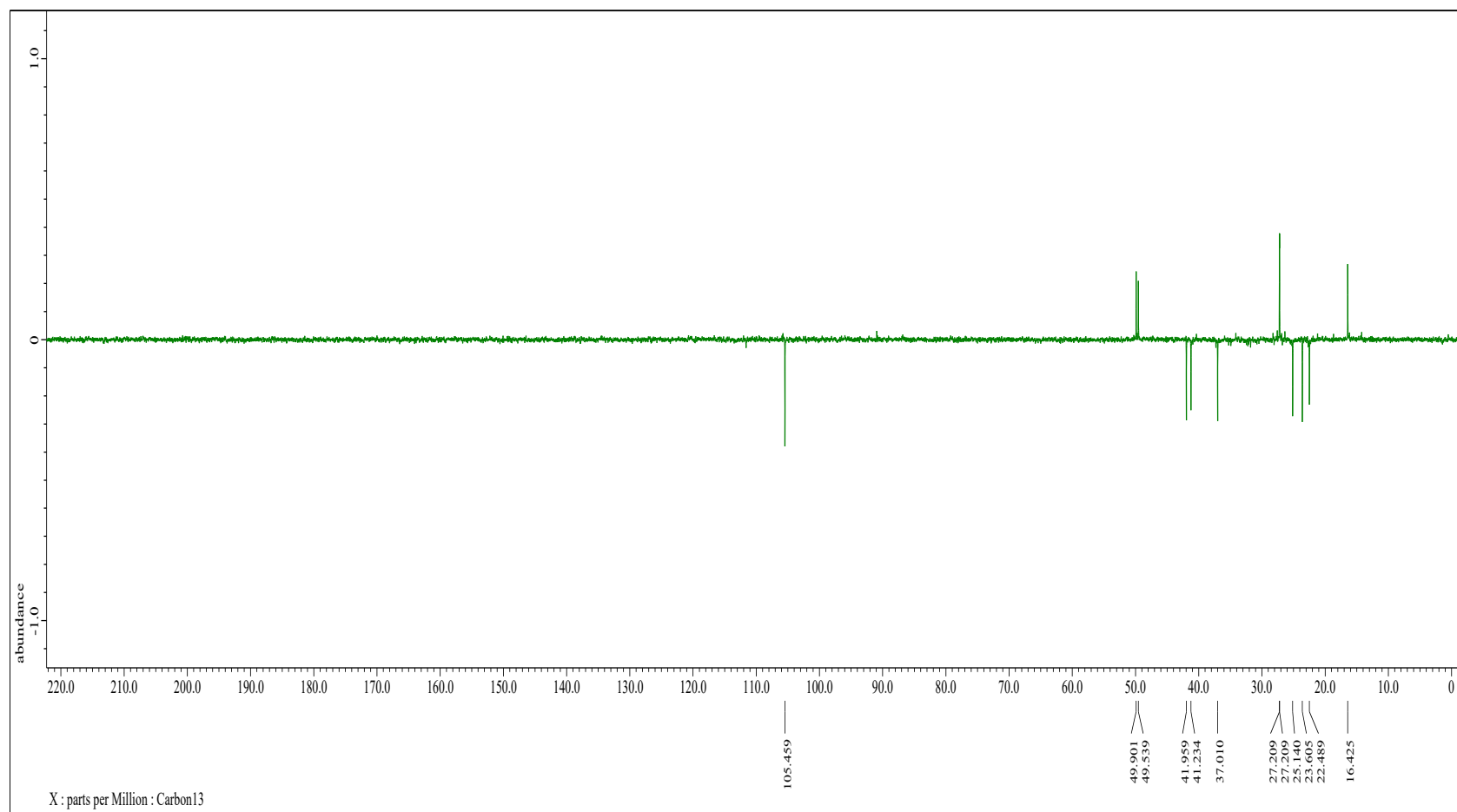


Figure S36. DEPT spectrum of **8** (Recorded in CDCl₃)

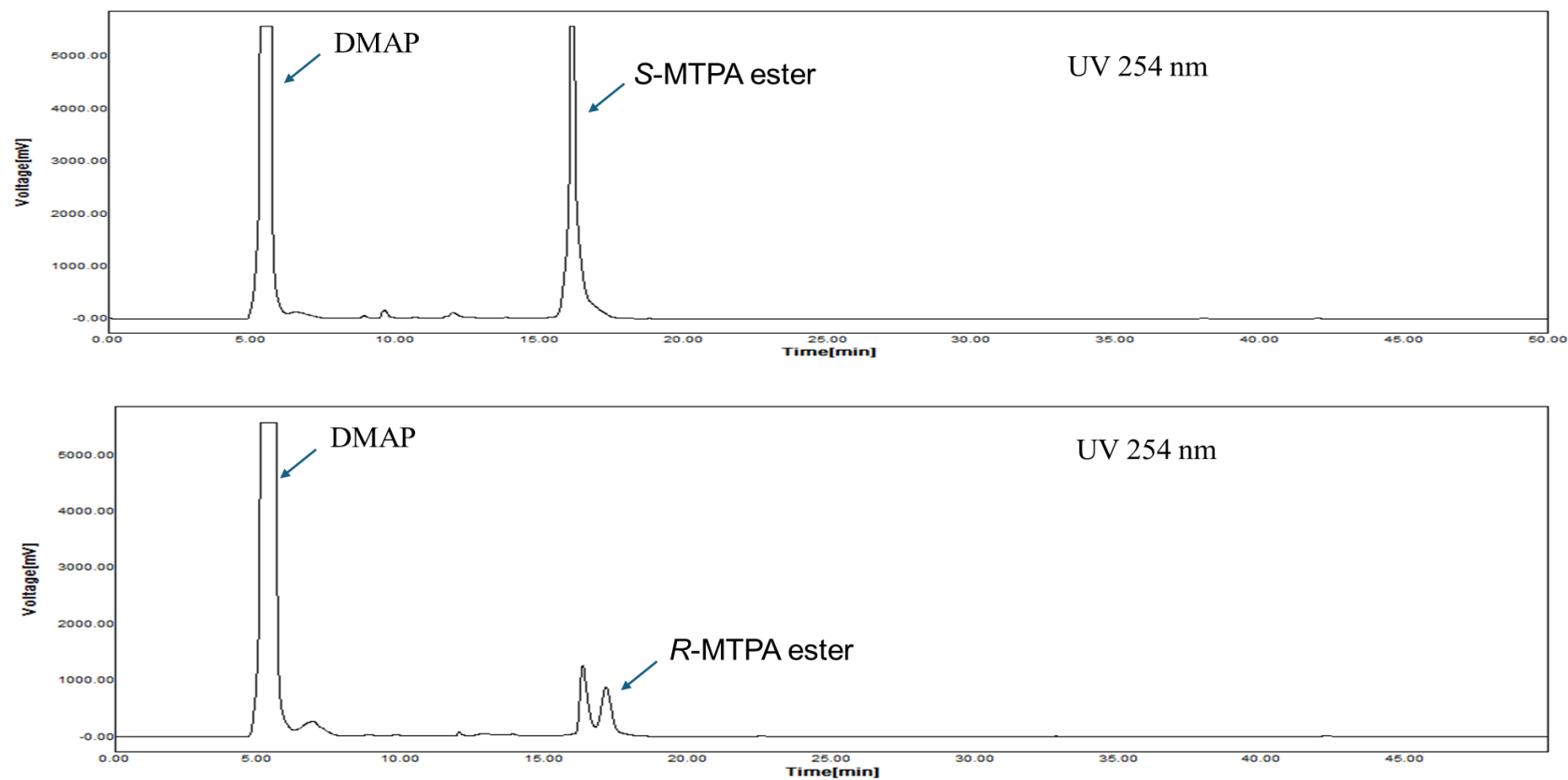


Figure S37. Chromatography Profile of (S) and R-MTPA ester

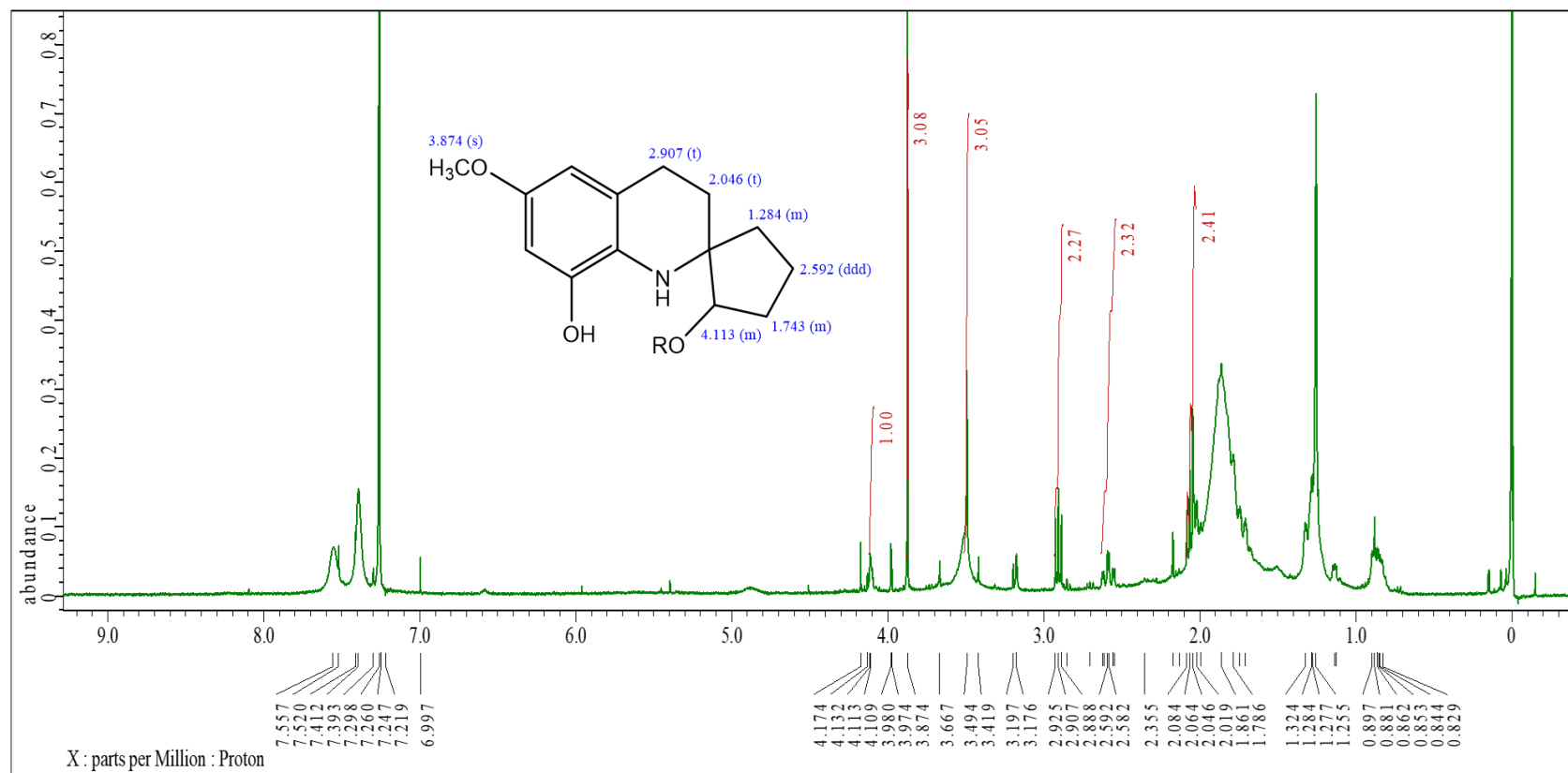


Figure S38. ¹H NMR spectrum of **1S** (Recorded in CDCl₃)

¹H NMR (CDCl₃, 400 MHz) of (*S*)-MTPA ester of **1**: δ_{H} 4.113(*m*, H-2), 1.743 (*m*, H-3), 2.592 (*dd*, $J = 4.4, 13.6, 18.0$ Hz, H-4), 1.284 (*m*, H-5), 2.046 (*t*, $J = 7.2$ Hz, H-3'), 2.907 (*t*, $J = 7.2$ Hz, H-4'), 6.977 (*s*, H-5'), 7.519 (*s*, H-7'), 3.874 (*s*, OCH₃).

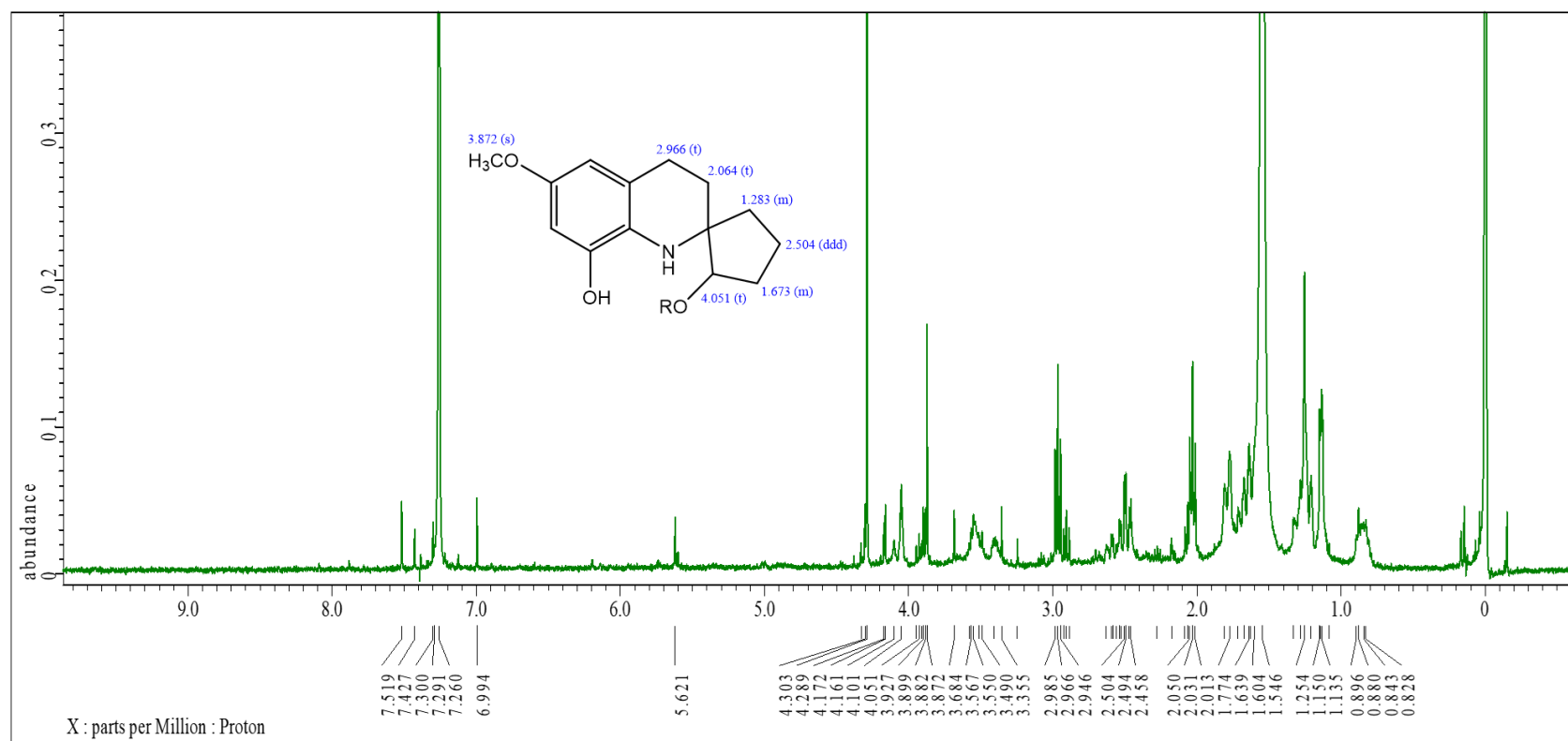


Figure S39. ^1H NMR spectrum of **1R** (Recorded in CDCl_3)

^1H NMR (CDCl_3 , 400 MHz) of (R) -MTPA ester of **1**: δ_{H} 4.051 (t, $J = 3.2$ Hz, H-2), 1.63 (m, H-3), 2.504 (dd, $J = 4.0, 13.6, 17.6$ Hz, H-4), 1.283 (m, H-5), 2.064 (t, $J = 7.2$ Hz, H-3'), 2.966 (t, $J = 7.2$ Hz, H-4'), 6.974 (s, H-5'), 7.519 (s, H-7'), 3.872 (s, OCH_3).

Reference

- [1]. Y. Wakahara, T. Noro, J. Sakata, H. Ueda, and H. Tokuyama (2022). Construction of Tetrahydroquinolines with spirocyclic structures at the 4-position, *Heterocycles*. **105**, 438-460.